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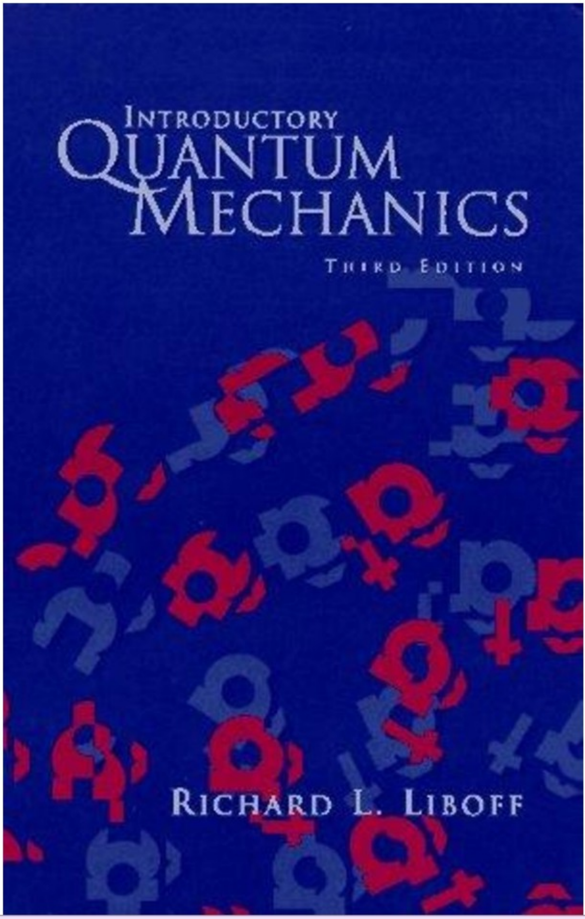
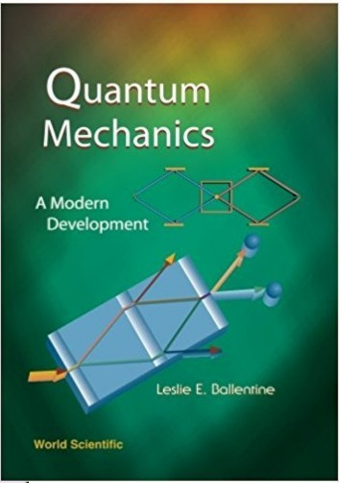
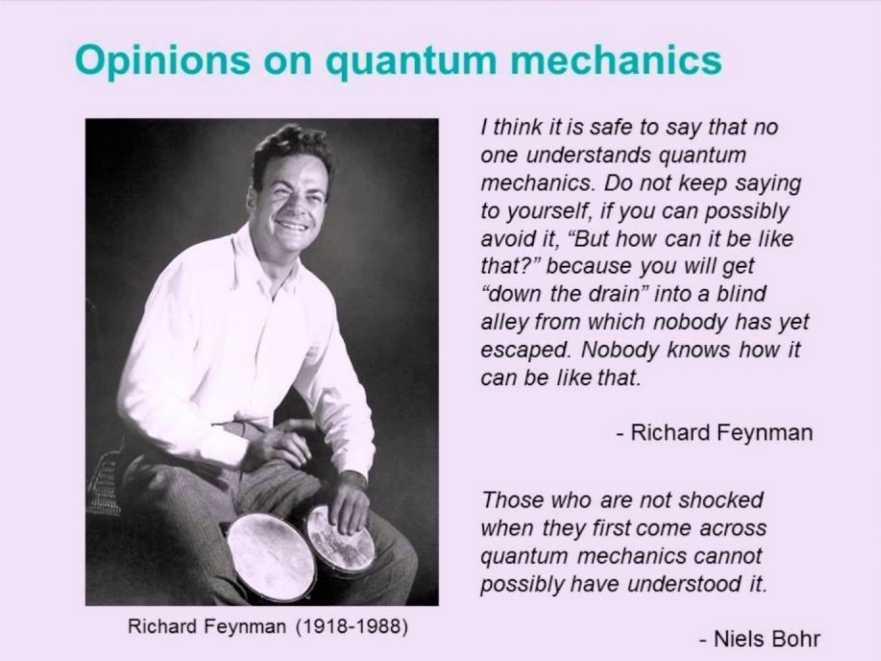






Opinions on quantum mechanics

I think it is safe to say that no one understands quantum mechanics. Do not keep saying to yourself, if you can possibly avoid it, “But how can it be like that?” because you will get “down the drain” into a blind alley from which nobody has yet escaped. Nobody knows how it can be like that.

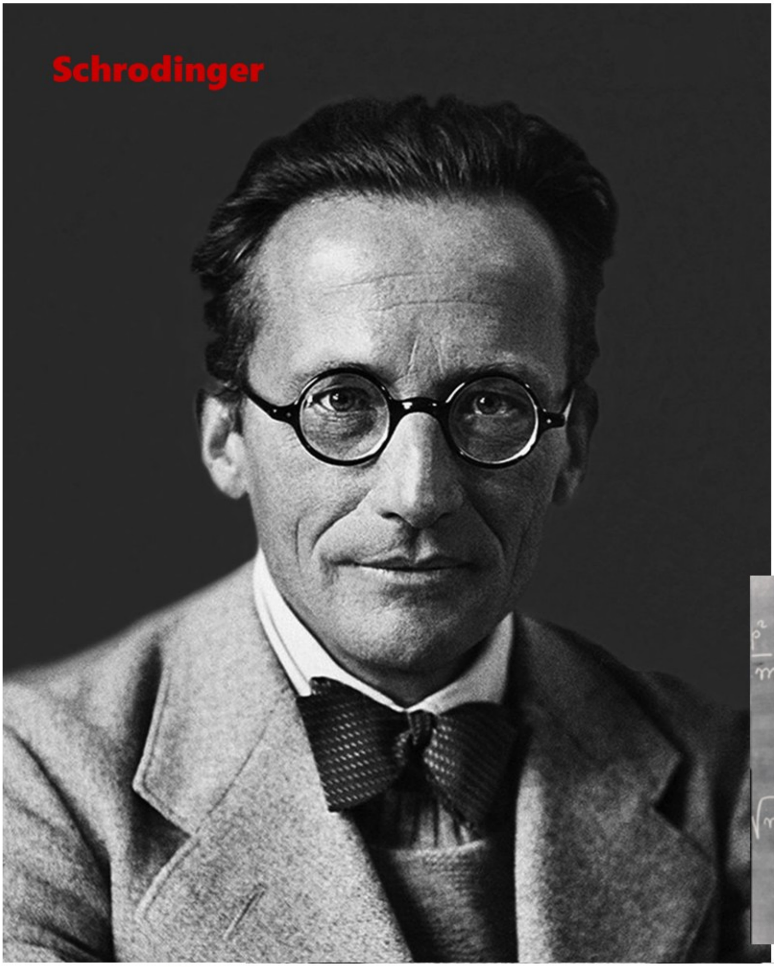
- Richard Feynman

Those who are not shocked when they first come across quantum mechanics cannot possibly have understood it.

- Niels Bohr

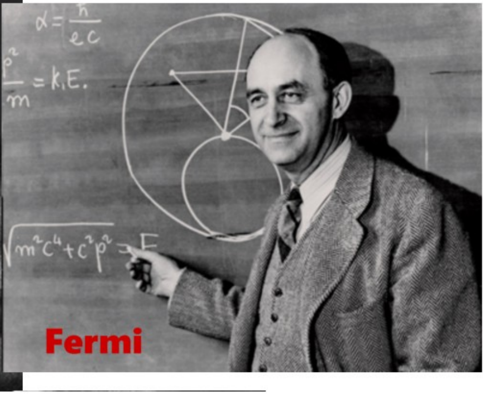
Richard Feynman (1918-1988)

Schrodinger



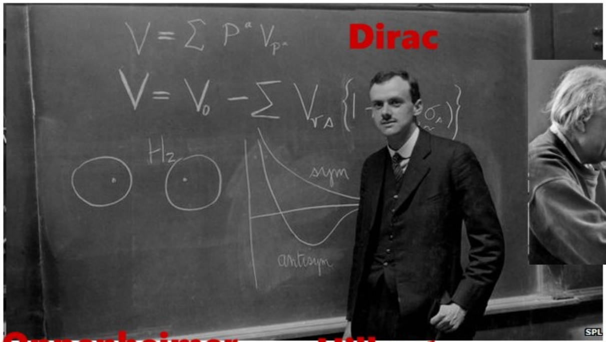
De Broglie

Fermi



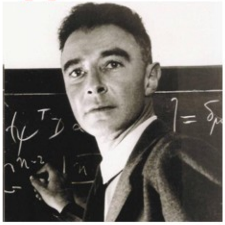
Heisenberg

Dirac

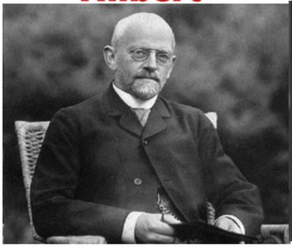


Einstein

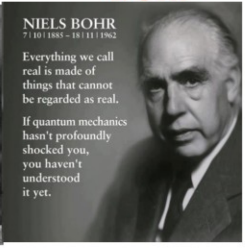
Oppenheimer



Hilbert



Bohr



NIELS BOHR
7 | 10 | 1885 – 18 | 11 | 1962

Everything we call real is made of things that cannot be regarded as real.

If quantum mechanics hasn't profoundly shocked you, you haven't understood it yet.

When we Look (Po.1 how, Po.2 What, Po.3 Why) we see?
by $\hat{A}$ a $\exists$ ψ

What is Generated?

CHAPTER 3

THE POSTULATES OF QUANTUM MECHANICS. OPERATORS, EIGENFUNCTIONS, AND EIGENVALUES

Why we see something here? be cause
"here exist" something not seen $\equiv \psi$..

why we receive

Reveuler 3.1 *Observables and Operators* how to receive
(a) Generated 3.2 *Measurement in Quantum Mechanics* revealed received
Thought 3.3 *The State Function and Expectation Values* what is available
Container 3.4 *Time Development of the State Function* Space Revealer
3.5 *Solution to the Initial-Value Problem in Quantum Mechanics*

Physics is readily-available revealed operators,
when mathematically the operators are derived we trace
the cause for the revelation before Physics is generated.

In this chapter we consider four basic postulates of quantum mechanics, which when taken with the Born postulate described in Section 2.8, serve to formalize the rules of quantum mechanics. Mathematical concepts material to these postulates are developed along with the physics. The postulates are applied over and over again throughout the text. We choose the simplest problems first to exhibit their significance and method of application—that is, problems in one dimension.

3.1 OBSERVABLES AND OPERATORS

Postulate I

This postulate states the following: To any self-consistently and well-defined observable in physics (call it A), such as linear momentum, energy, mass, angular momentum, or number of particles, there corresponds an operator (call it $\hat{A}$) such that measurement of A yields values (call these measured values a) which are eigenvalues of $\hat{A}$. That is, the values, a, are those values for which the equation

$$\hat{A}\varphi = a\varphi \qquad \boxed{\text{an eigenvalue equation}} \tag{3.1}$$

for any direct output
φ intrensic state

This eqtn reveals all the φ's satisfing it.

TABLE 3.1 Examples of operators

$\hat{D} = \partial/\partial x$	$\hat{D}\varphi(x) = \partial\varphi(x)/\partial x$
$\hat{\Delta} = -\partial^2/\partial x^2 = -\hat{D}^2$	$\hat{\Delta}\varphi(x) = -\partial^2\varphi(x)/\partial x^2$
$\hat{M} = \partial^2/\partial x\, \partial y$	$\hat{M}\varphi(x, y) = \partial^2\varphi(x, y)/\partial x\, \partial y$
$\hat{I}$ = operation that leaves φ unchanged	$\hat{I}\varphi = \varphi$
$\hat{Q} = \int_0^1 dx'$	$\hat{Q}\varphi(x) = \int_0^1 dx'\varphi(x')$
$\hat{F}$ = multiplication by $F(x)$	$\hat{F}\varphi(x) = F(x)\varphi(x)$
$\hat{B}$ = division by the number 3	$\hat{B}\varphi(x) = \frac{1}{3}\varphi(x)$
$\hat{\Theta}$ = operator that annihilates φ	$\hat{\Theta}\varphi = 0$
$\hat{P}$ = operator that changes φ to a specific polynomial of φ	$\hat{P}\varphi = \varphi^3 - 3\varphi^2 - 4$
$\hat{G}$ = operator that changes φ to the number 8	$\hat{G}\varphi = 8$

has a solution φ. The function φ is called the *eigenfunction* of $\hat{A}$ corresponding to the eigenvalue a.

Examples of mathematical operators, which are not necessarily connected to physics, are offered in Table 3.1. (Labels such as D, G, and M are of no special significance.) An operator operates on a function and makes it something else (except for the identity operator $\hat{I}$).

Let us now turn to operators that correspond to physical observables. Two very important such observables are the momentum and the energy.

The Momentum Operator $\hat{\mathbf{p}}$

The operator that corresponds to the observable linear momentum is

$$\hat{\mathbf{p}} = -i\hbar\nabla \tag{3.2}$$

What are the eigenfunctions and eigenvalues of the momentum operator? Consider that the particle (whose momentum is in question) is constrained to move in one dimension (x). Then the momentum has only one nonvanishing component, p_x. The corresponding operator is

$$\hat{p}_x = -i\hbar\frac{\partial}{\partial x} \tag{3.3}$$

The eigenvalue equation for this operator is

$$-i\hbar\frac{\partial}{\partial x}\varphi = p_x\varphi \tag{3.4}$$

The values p_x represent the *only* possible values that measurement of the x component of momentum will yield. The eigenfunction $\varphi(x)$ corresponding to a specific value of momentum (p_x) is such that $|\varphi|^2\,dx$ is the probability of finding the particle (with momentum p_x) in the interval $x, x + dx$. Suppose we stipulate that the particle is a *free* particle. It is unconfined (along the x axis). For this case there is no boundary condition on φ and the solution to (3.4) is

$$\varphi = A \exp\left(\frac{ip_x x}{\hbar}\right) = Ae^{ikx} \tag{3.5}$$

where we have labeled the wavenumber k and have deleted the subscript x.

$$k = \frac{p}{\hbar} \tag{3.6}$$

The eigenfunction given by (3.5) is a periodic function (in x). To find its wavelength λ, we set

$$\begin{gathered} e^{ikx} = e^{ik(x+\lambda)} \\ 1 = e^{ik\lambda} = \cos k\lambda + i \sin k\lambda \end{gathered} \tag{3.7}$$

which is satisfied if

$$\begin{gathered} \cos k\lambda = 1 \\ \sin k\lambda = 0 \end{gathered} \tag{3.8}$$

The first nonvanishing solution to these equations is

$$k\lambda = 2\pi \tag{3.9}$$

which (with 3.6) is equivalent to the de Broglie relation

$$p = \frac{h}{\lambda} \tag{3.10}$$

We conclude that the eigenfunction of the momentum operator corresponding to the eigenvalue p has a wavelength that is the de Broglie wavelength h/p.

In quantum mechanics it is convenient to speak in terms of wavenumber k instead of momentum p. In this notation one says that the eigenfunctions and eigenvalues of the momentum operator are

$$\varphi_k = Ae^{ikx}, \qquad p = \hbar k \tag{3.11}$$

The subscript k on φ_k denotes that there is a continuum of eigenfunctions and eigenvalues, $\hbar k$, which yield nontrivial solutions to the eigenvalue equation, (3.4).

The Energy Operator $\hat{H}$

The operator corresponding to the energy is the Hamiltonian $\hat{H}$, with momentum $\mathbf{p}$ replaced by its operator counterpart, $\hat{\mathbf{p}}$. For a single particle of mass m, in a potential field $V(\mathbf{r})$,

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\mathbf{r}) = -\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}) \tag{3.12}$$

The eigenvalue equation for $\hat{H}$,

$$\hat{H}\varphi(\mathbf{r}) = E\varphi(\mathbf{r}) \tag{3.13}$$

is called the *time-independent Schrödinger equation*. It yields the possible energies E which the particle may have. Again consider the free particle. The energy of a free particle is purely kinetic, so

$$\hat{H} = \frac{\hat{p}^2}{2m} = -\frac{\hbar^2}{2m}\nabla^2 \tag{3.14}$$

Constraining the particle to move in one dimension, the time-independent Schrödinger equation becomes

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\varphi = E\varphi \tag{3.15}$$

In terms of the wave vector

$$k^2 = \frac{2mE}{\hbar^2} \tag{3.16}$$

(3.15) appears as

$$\varphi_{xx} + k^2\varphi = 0 \tag{3.17}$$

The subscript x denotes differentiation. For a free particle there are no boundary conditions and we obtain[1]

$$\varphi = Ae^{ikx} \tag{3.18}$$

This is an eigenfunction of $\hat{H}$ which corresponds to the energy eigenvalue

$$E = \frac{\hbar^2 k^2}{2m} \tag{3.19}$$

We have found above (3.11) that the momentum of a free particle is $\hbar k$. This is clearly the same $\hbar k$ that appears in (3.19), since for a free particle

$$E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m} \tag{3.20}$$

---

[1] The general solution of (3.17) is discussed in Section 5.3.

3 We note also that the eigenfunction of $\hat{H}$, (3.18), is also an eigenfunction of $\hat{p}$ (3.11). That $\hat{H}$ and $\hat{p}$ for a free particle have common eigenfunctions is a special case of a more general theorem to be discussed later.[1] The following simple argument demonstrates this fact. Let

$$\hat{p}\varphi = \hbar k\varphi \tag{3.21}$$

Let us see if φ is also an eigenfunction of $\hat{H}$ (for a free particle).

$$\begin{aligned} \hat{H}\varphi &= \frac{\hat{p}}{2m}(\hat{p}\varphi) = \frac{\hat{p}(\hbar k\varphi)}{2m} = \frac{\hbar k}{2m}\hat{p}\varphi \\ &= \frac{(\hbar k)^2}{2m}\varphi \end{aligned} \tag{3.22}$$

It follows that φ is also an eigenfunction of $\hat{H}$.

-1 Both the energy and momentum eigenvalues for the free particle comprise a continuum of values:

$$\boxed{E = \frac{\hbar^2 k^2}{2m} \qquad p = \hbar k} \tag{3.23}$$

That is, these are valid eigenvalues for *any* wavenumber k. The eigenfunction (of both $\hat{H}$ and $\hat{p}$) corresponding to these eigenvalues is

$$\varphi_k = Ae^{ikx} \tag{3.24}$$

1 If the free particle is in this state, measurement of its momentum will definitely yield $\hbar k$, and measurement of its energy will definitely yield $(\hbar^2 k^2/2m)$.

-2 Suppose that we measure its position x; what do we find? Well, where is the particle most likely to be? Again we call on the Born postulate. If the particle is in the state φ_k, the probability density relating to the probability of finding the particle in the interval x, $x + dx$, is

$$|\varphi_k|^2 = |A|^2 = \text{constant} \tag{3.25}$$

The probability density is the same constant value for all x. That means we would be equally likely to find the particle at any point from $x = -\infty$ to $x = +\infty$. This is a statement of maximum uncertainty which is in agreement with the Heisenberg uncertainty principle. In the state φ_k, it is known with absolute certainty that measurement of momentum yields $\hbar k$. Therefore, for the state φ_k, $\Delta p = 0$, whence $\Delta x = \infty$.

2 We mentioned in Section 2.7 that E and t are complementary variables; that is, they obey the relation $\Delta E\,\Delta t \geq \hbar$. Specifically, this means that if the energy is uncertain by amount ΔE, *the time it takes to measure* E is uncertain by $\Delta t \geq \hbar/\Delta E$. Now for the problem at hand, in the state φ_k, it is certain that measurement of E yields $\hbar k^2/2m$.

---

[1] The commutator theorem, Chapter 5.

3.4 If the eigenfn^{ns} of $\hat{\mathcal{D}}$ are of the form $\phi_\beta = e^{\beta x} g(x)$, $\Rightarrow$ $\beta \in \mathbb{C}$

$\hat{\mathcal{D}}\,\phi_\beta = \lambda\,\phi_\beta$ where λ is the eigenvalue of $\hat{\mathcal{D}}$,

$\hat{\mathcal{D}}\,(e^{\beta x}\, g(x)) = \hat{\mathcal{D}}\, h(x) = e^{\beta(x+\varepsilon)}\, g(x+\varepsilon) = e^{\beta(x+\varepsilon)}\, g(x)$

$= e^{\beta\varepsilon}\,(e^{\beta x}\, g(x)) = e^{\beta\varepsilon}\, h(x) \Rightarrow \hat{\mathcal{D}}\, h(x) = e^{\beta\varepsilon}\, h(x)$

Which is an eigenvalue eqt^{n} $h(x) = \phi_\beta(x) = e^{\beta x}\, g(x)$.

3 Therefore, $\Delta E = 0$. To measure E we have to let the particle interact with some sort of energy-measuring apparatus, say a plate with a spring attached to measure the momentum imparted to the plate when the particle hits it head on. Well, if the plate † 3· with attached spring is placed in the path of the particle, how long must we wait before we detect something? We can wait 10^{-8} s—or we can wait 10^{10} yr. The uncertainty Δt is infinite in the present case, since there is an infinite uncertainty in Δx.

PROBLEMS

3.1 For each of the operators listed in Table 3.1 ($\hat{D}, \hat{\Delta}, \hat{M}$, etc.), construct the square, that is, $\hat{D}^2, \hat{\Delta}^2, \ldots$.

Answer (partial)

$$\hat{I}^2\varphi = \hat{I}\varphi = \varphi$$

$$\hat{Q}^2\varphi = \hat{Q}\int_0^1 dx'\varphi(x') = \int_0^1 dx'' \int_0^1 dx'\varphi(x')$$

$$\hat{F}^2\varphi = F^2\varphi$$

$$\hat{B}^2\varphi = \tfrac{1}{9}\varphi$$

$$\hat{P}^2\varphi = \hat{P}(\hat{P}\varphi) = (\varphi^3 - 3\varphi^2 - 4)^3 - 3(\varphi^3 - 3\varphi^2 - 4)^2 - 4$$

3.2 The inverse of an operator $\hat{A}$ is written $\hat{A}^{-1}$. It is such that

$$\hat{A}^{-1}\hat{A}\varphi = \hat{I}\varphi = \varphi$$

Construct the inverses of $\hat{D}, \hat{I}, \hat{F}, \hat{B}, \hat{\Theta}, \hat{G}$, provided that such inverses exist.

3.3 An operator $\hat{O}$ is *linear* if

$$\hat{O}(a\varphi_1 + b\varphi_2) = a\hat{O}\varphi_1 + b\hat{O}\varphi_2$$

where a and b are arbitrary constants. Which of the operators in Table 3.1 are linear and which are nonlinear?

† **3.4** The displacement operator $\hat{\mathscr{D}}$ is defined by the equation

$$\hat{\mathscr{D}}f(x) = f(x + \zeta)$$

Show that the eigenfunctions of $\hat{\mathscr{D}}$ are of the form

$$\varphi_\beta = e^{\beta x}g(x)$$

where

$$g(x + \zeta) = g(x)$$ Periodic fn

and β is any complex number. What is the eigenvalue corresponding to φ_β?

3.5 An electron moves in the x direction with de Broglie wavelength 10^{-8} cm.

(a) What is the energy of the electron (in eV)?

(b) What is the time-independent wavefunction of the electron?

3.2 MEASUREMENT IN QUANTUM MECHANICS

Postulate II

The events that happen only by the time of "measurement"

The second postulate[1] of quantum mechanics is: measurement of the observable A that yields the value a leaves the system in the state φ_a, where φ_a is the eigenfunction of $\hat{A}$ that corresponds to the eigenvalue a.

1 As an example, suppose that a free particle is moving in one dimension. We do not know which state the particle is in. At a given instant we measure the particle's momentum and find the value $p = \hbar k$ (with k a specific value, say 1.3×10^{10} cm^{-1}). This measurement[2] throws the particle into the state φ_k, so immediate subsequent measurement of p is certain to yield $\hbar k$.

2 Suppose that one measures the position of a free particle and the position $x = x'$ is measured. The first two postulates tell us the following. (1) There is an operator corresponding to the measurement of position, call it $\hat{x}$. (2) Measurement of x that yields the value x' leaves the particle in the eigenfunction of $\hat{x}$ corresponding to the eigenvalue x'.

The operator equation appears as

$$\hat{x}\delta(x - x') = x'\delta(x - x') \tag{3.26}$$

Dirac Delta Function

The eigenfunction of $\hat{x}$ has been written[3] $\delta(x - x')$ and is called the *Dirac delta function*. It is defined in terms of the following two properties. The first are the integral properties

$$\langle x|\varphi\rangle = \int_{-\infty}^{\infty} f(x')\delta(x - x')\,dx' = f(x)$$

$$\int_{-\infty}^{\infty} \delta(x - x')\,dx' = 1 \tag{3.27}$$

---

[1] This postulate has been the source of some discussion among physicists. For further reference, see B. S. DeWitt. *Phys. Today* 23, 30 (September 1970).

[2] Measurement is taken in the idealized sense. More formal discussions on the theory of measurement may be found in K. Gottfried, *Quantum Mechanics*, W. A. Benjamin, New York, 1966; J. Jauch, *Foundations of Quantum Mechanics*, Addison-Wesley, Reading, Mass., 1968, and E. C. Kemble, *The Fundamental Principles of Quantum Mechanics with Elementary Applications*, Dover, New York, 1958.

[3] More accurately one says that $\delta(x - x')$ is an eigenfunction of $\hat{x}$ in the coordinate representation. This topic is returned to in Section 7.4 and in Appendix A.

$\hat{A}\psi = a\psi$, a is the "received Information" from the observable

A which is in the same space of ψ as the observer.

or equivalently, in terms of the single variable y

$$\int_{-\infty}^{\infty} f(y)\delta(y)\,dy = f(0) \tag{3.28}$$

$$\int_{-\infty}^{\infty} \delta(y)\,dy = 1$$

The second defining property is the value

$$\delta(y) = 0 \qquad (\text{for } y \neq 0) \tag{3.29}$$

A sketch of $\delta(y)$ is given in Fig. 3.1. Properties of $\delta(y)$ are usually proved with the aid of the defining integral (3.27). For instance, consider the relation

$$y\delta'(y) = -\delta(y) \tag{3.30}$$

To establish this relation we employ a *test function* $f(y)$ and perform the following integration by parts.

$$\begin{aligned}\int_{-\infty}^{\infty} f(y)y\delta'(y)\,dy &= \int_{-\infty}^{\infty} \frac{d}{dy}(fy\delta)\,dy - \int_{-\infty}^{\infty} \delta\frac{d}{dy}(yf)\,dy \\ &= -\int_{-\infty}^{\infty} \delta(y)\left(y\frac{df}{dy} + f\right)dy = -\int_{-\infty}^{\infty} \delta(y)f(y)\,dy\end{aligned} \tag{3.31}$$

which establishes (3.30).

The student should not lose sight of the fact that $\hat{x}$, when operating on a function $f(x)$, merely represents multiplication by x. For example, $\hat{x}f(x) = xf(x)$. It is only with regard to its own eigenvalue problem that $\hat{x}$ assumes a somewhat more abstract quality. These topics will be returned to in Chapter 11 and discussed further in Appendix A.

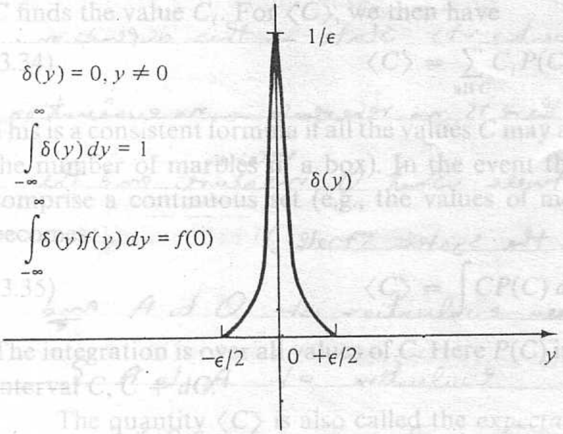

$1/\epsilon$
$\delta(y) = 0,\ y \neq 0$
$\int_{-\infty}^{\infty} \delta(y)\,dy = 1$
$\delta(y)$
$\int_{-\infty}^{\infty} \delta(y)f(y)\,dy = f(0)$
$-\epsilon/2$
0
$+\epsilon/2$
y

FIGURE 3.1 **Dirac delta function $\delta(y)$. The curve is distorted to bring out essential features. A more accurate picture is obtained in the limit $\epsilon \to 0$.**

PROBLEMS

3.6 Establish the following properties of $\delta(y)$.

(a) $\delta(y) = \delta(-y)$

(b) $\delta'(y) = -\delta'(-y)$

(c) $y\delta(y) = 0$

(d) $\delta(ay) = a^{-1}\,\delta(y)$

(e) $\delta(y^2 - a^2) = (2a)^{-1}[\delta(y-a) + \delta(y+a)]$

(f) $\displaystyle\int_{-\infty}^{\infty} \delta(a-y)\,\delta(y-b)\,dy = \delta(a-b)$

(g) $f(y)\,\delta(y-a) = f(a)\,\delta(y-a)$

(h) $y\,\delta'(y) = -\delta(y)$

(i) $\displaystyle\int g(y)\,\delta[f(y)-a]\,dy = \left.\frac{g(y)}{df/dy}\right|_{\substack{y=y_0\\ f(y_0)=a}}$

3.7 Show that the following are valid representations of $\delta(y)$:

(a) $\displaystyle 2\pi\delta(y) = \int_{-\infty}^{\infty} e^{iky}\,dk$

(b) $\displaystyle \pi\delta(y) = \lim_{\eta\to\infty} \frac{\sin \eta y}{y}$

Note: In mathematics, an object such as $\delta(y)$; which is defined in terms of its integral properties, is called a *distribution.* Consider all $\chi(y)$ defined on the interval $(-\infty, \infty)$ for which

$$\int_{-\infty}^{\infty} |\chi(y)|^2\,dy < \infty$$

Then two distributions, δ_1 and δ_2, are *equivalent* if for all $\chi(y)$,

$$\int_{-\infty}^{\infty} \chi\,\delta_1\,dy = \int_{-\infty}^{\infty} \chi\,\delta_2\,dy$$

When one establishes that a mathematical form such as $\int_{-\infty}^{\infty} \exp(iky)\,dy$ is a representation of $\delta(y)$, one is in effect demonstrating that these two objects are *equivalent as distributions.*

3.8 Show that the continuous set of eigenfunctions $\{\delta(x-x')\}$ obeys the "orthonormality" condition

$$\int_{-\infty}^{\infty} \delta(x-x')\,\delta(x-x'')\,dx = \delta(x'-x'')$$

3.9 (a) Show that $\delta(\sqrt{x}) = 0$.

(b) Evaluate $\delta(\sqrt{x^2 - a^2})$.

(a) $\delta(y) = \delta(-y) \Rightarrow \int_{-\infty}^{\infty}\delta(y)\,dy = 1 \Rightarrow$ replace y by $(-t)$ $\Rightarrow$

$-\int_{+\infty}^{-\infty}\delta(-t)\,d(-t) = \boxed{-x-}\int_{-\infty}^{\infty}\delta(-t)\,d(-t) = 1 = \int_{-\infty}^{\infty}\delta(-y)\,d(-y)$

Let $(-y) = x \Rightarrow 1 = \int_{-\infty}^{\infty}\delta(x)\,dx = \int_{-\infty}^{\infty}\delta(y)\,dy$ both x & y are dummy variables $\Rightarrow \delta(x) = \delta(y)$ when $x = -y \Rightarrow \delta(y) = \delta(-y)$

(b) Since $\delta(y) = \delta(-y) \Rightarrow \frac{d}{dy}\delta(y) = \frac{d}{dy}\delta(-y) = \frac{d}{dx}\delta(x)\frac{dx}{dy} = -\delta'(-y) = \delta(y)$

(c) Since $\delta(y) = 0$ ∀ $y \neq 0 \Rightarrow y\,\delta(y) = 0$ ∀ $y \neq 0$
but if $y = 0 \Rightarrow$ still $y\,\delta(y) = 0$.

(d) $\frac{1}{a}\int_{-\infty}^{\infty}\delta(ay)\,d(ay) = \frac{1}{a}\int_{-\infty}^{\infty}\delta(t)\,dt = 1$ $a^{-1}\delta(-y)$

(e) $\delta(y^2-a^2) = \delta[y(y-a) + a(y-a)] =$

✓ (f) $\int_{-\infty}^{\infty}\delta(a-y)\,\delta(y-b)\,dy = \int_{-\infty}^{\infty}\langle a|y\rangle\langle y|b\rangle\,dy = \langle a|I|b\rangle = \langle a|b\rangle = \delta(a-b)$

(g) $\int_{-\infty}^{\infty}\delta(y-a)f(y)\,dy = \int_{-\infty}^{\infty}\langle a|y\rangle\langle y|f\rangle\,dy = \langle a|I|f\rangle = \langle a|f\rangle = f(a)$

(i) $\int g(y)\,\delta[f(y)-a]\,dy = \int g(y)\,\delta(f-a)\,(df/dy)^{-1}\,df = \int\left(\frac{g(y)}{df/dy}\right)\delta(f-a)\,df$

$\int\left(\frac{g(y)}{f'(y)}\right)\delta(f-a)\,df = \int h(y)\,\delta(f-a)\,df = \int\delta(f-a)\,h(y)\,df =$

$\int\delta(f-a)\,h(y)\,df = \langle a|h\rangle = h(a, f(y)=a) = \left.\frac{g(y)}{df/dy}\right|_{\substack{y=y_0\\ f(y_0)=a}}$

measures

1 Can a System observes or evaluates its State → this depends on:

$\hat{A}$, a, φ_a → $\boxed{\text{w.r}}$ to what ≡ if there is no reference → no evaluation

receives

Is there a Contradiction between what O measures and the (actual intrensic state w.r to the system itself)

≡ What is the relation between evaluation of O to A and evaluation of A to A?
(at the time of measurement)

2 What is the relation between φ and the eigenstates (φ_a)?

φ depends indirectly on $\hat{A}$ only through $\sum_{\forall a} b_a\,\varphi_a$, where $\hat{A}\varphi_a = a\,\varphi_a$

Both the observer O and the Observable A are physical w.r to O i.e O, A ∈ Physics. Thus before saying that we observe A, O must ask, what is so special about A that enables O to observe A, this abstract question Constitutes the heart of what is meant by a physics or physical which will lead O to the abstract object which is ψ, having operated on it by the "physics revealer operator", generates to O the Observable system A in any (time) depending on when O set the Observation, hence what is received from A, by O, is a. The physics revealer operator is determined by O who wants A to be revealed to him => this Physics revealer operator is $\hat{A}$. But reveal what, and why there is an object hidden that is needed to be revealed, => What $\mapsto \psi_A$ and Why $\mapsto \psi_A$ is a mathematical object, and the meaning is Contained in the word mathematical, and what is implied by mathematics; is not the Conventional view to it as eqtns, theorems, and definitions. No, mathematics is as real as physics is real to us, but it is a world in each physics, that is in a need to a revealer to generate physics.

Any physics Contains a mathematics and
any mathematics Contains a Logic,
and Existance or Reality is solved by Logic to Logic. $O\,(\xrightarrow{\text{revealer}})$

It is possible to find a mathematical structure that is not revealed in the physics, only in the head of man.

* With respect to the observer physics is generated Logic and mathematics is to be revealed Logic.

3.3 THE STATE FUNCTION AND EXPECTATION VALUES

Postulate III

The third postulate of quantum mechanics establishes the existence of the state function and its relevance to the properties of a system: The state of a system at any instant of time may be represented by a state or wave function ψ which is continuous
† and differentiable. All information regarding the state of the system is contained in the wavefunction. Specifically, if a system is in the state $\psi(\mathbf{r}, t)$, the average of any physical observable C relevant to that system at time t is

$\psi = \forall t$ available

$$\langle\psi|\hat{C}|\psi\rangle = \langle C\rangle = \int \psi^* \hat{C} \psi \, d\mathbf{r} \tag{3.32}$$

global state

(The differential of volume is written $d\mathbf{r}$.) The average, $\langle C\rangle$, is called the *expectation value* of C.

1 The physical meaning of the average of an observable C involves the following type of (conceptual) measurements. The observable C is measured in a specific experiment, X. One prepares a very large number (N) of identical replicas of X. The initial states $\psi(\mathbf{r}, 0)$ in each such replica are all identical. At the time t, one measures C in all these replica experiments and obtains the set of values $C_1, C_2, \ldots, C_N$. The average of C is then given by the rule

$$\langle C\rangle = \frac{1}{N}\sum_{i=1}^{N} C_i \qquad (N \gg 1) \tag{3.33}$$

2 The postulate stated above claims that this experimentally calculated average (3.33) is the same as that given by the integral in (3.32). Another way of defining $\langle C\rangle$ is in terms of the probability $P(C_i)$. This function gives the probability that measurement of C finds the value C_i. For $\langle C\rangle$, we then have

$$\langle C\rangle = \sum_{\text{all } C} C_i P(C_i) \tag{3.34}$$

2 This is a consistent formula if all the values C may assume comprise a discrete set (e.g., the number of marbles in a box). In the event that the values that C may assume comprise a continuous set (e.g., the values of momentum of a free particle), $\langle C\rangle$ becomes

$$\langle C\rangle = \int C P(C) \, dC \tag{3.35}$$

The integration is over all values of C. Here $P(C)$ is the probability of finding C in the interval C, $C + dC$.

3 The quantity $\langle C\rangle$ is also called the *expectation value* of C because it is representative of the value one expects to obtain in any given measurement of C. This will

be especially true if the deviation of values of C from the mean value $\langle C\rangle$ is not large. As discussed in Section 2.7, a measure of this spread of values about the value $\langle C\rangle$ is given by the mean-square deviation ΔC, defined through

$$(\Delta C)^2 = \langle (C - \langle C\rangle)^2\rangle = \langle C^2\rangle - \langle C\rangle^2 \tag{3.36}$$

In order to become familiar with the operational use of postulate III, we work out the following one-dimensional problem. A particle is known to be in the state

$$\psi(x, t) = A \exp\left[\frac{-(x-x_0)^2}{4a^2}\right] \exp\left(\frac{ip_0 x}{\hbar}\right) \exp(i\omega_0 t) \tag{3.37}$$

The lengths x_0 and a are constants, as are the momentum p_0 and frequency ω_0. The (real) constant A is determined through normalization. This then ensures that $\psi^*\psi$ is a numerically correct probability density.

$$\begin{gathered}\int_{-\infty}^{\infty} |\psi|^2\, dx = A^2 a \int_{-\infty}^{\infty} e^{-\eta^2/2}\, d\eta = \sqrt{2\pi}\, A^2 a = 1 \\ A^2 = \frac{1}{a\sqrt{2\pi}}\end{gathered} \tag{3.38}$$

The nondimensional "dummy" variable η and constant η_0 are such that

$$\begin{gathered}\eta = \frac{x - x_0}{a} \\ x = a(\eta + \eta_0) \\ \eta_0 = \frac{x_0}{a}\end{gathered} \tag{3.39}$$

Having obtained A, we may now calculate the expectation of x:

$$\begin{aligned}\langle x\rangle &= \int_{-\infty}^{\infty} \psi^* \hat{x} \psi\, dx = \int_{-\infty}^{\infty} \psi^* x \psi\, dx \\ &= A^2 a^2 \int_{-\infty}^{\infty} e^{-\eta^2/2}(\eta + \eta_0)\, d\eta = a\eta_0 \left(aA^2 \int_{-\infty}^{\infty} e^{-\eta^2/2}\, d\eta \right)\end{aligned} \tag{3.40}$$

which, with the normalization condition (3.38), gives

$$\langle x\rangle = a\eta_0 = x_0 \tag{3.41}$$

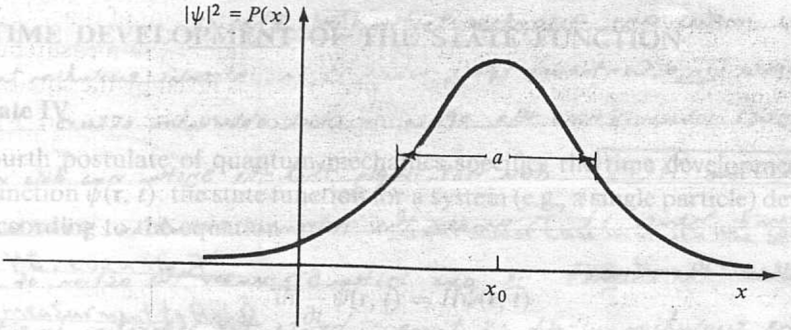


FIGURE 3.2 Gaussian probability density with variance a^2. The variance measures the spread of $P(x)$ about the mean, $\langle x \rangle = x_0$. In quantum mechanics the square root of variance a is called the uncertainty in x and is denoted as Δx, so for the case under discussion,

$$a = \Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$$

[Note that integration of the odd integrand $\eta \exp(-\eta^2)$ in (3.40) vanishes.] That x_0 is the proper value for $\langle x \rangle$ is evident from the sketch of $|\psi|^2$ shown in Fig. 3.2.

If we call

$$|\psi|^2 \, dx = P(x) \, dx \tag{3.42}$$

the probability of finding the particle in the interval x, $x + dx$, then

$$\langle x \rangle = \int_{-\infty}^{\infty} x P(x) \, dx \tag{3.43}$$

This is consistent with definition (3.35).

The probability density

$$P(x) = \frac{1}{a\sqrt{2\pi}} \exp\left[\frac{-(x - x_0)^2}{2a^2}\right]$$

is called the *Gaussian* or *normal distribution*, and a^2 is called the *variance* of x. It is a measure of the spread of $P(x)$ about the mean value

$$\langle x \rangle = x_0$$

As shown in Problem 3.10, the variance of x is the same as the mean-square deviation, $(\Delta x)^2$.

$$(\Delta x)^2 = \langle x^2 \rangle - \langle x \rangle^2 = a^2 + x_0{}^2 - x_0{}^2 = a^2$$

If it is known that a particle is in the state $\psi(x)$ at a given instant of time, and that in this state, $\langle x \rangle = x_0$, one may then ask: With what certainty will measurement of x find the value x_0? A measure of the relative *uncertainty* is given by the square root of the variance, Δx. If this value is large (compared to $\langle x \rangle$), one may say with little certainty that measurement will find the particle at x_0. If, on the other hand, Δx is small, one is more certain that measurement will find the particle at $x = x_0$. In quantum mechanics Δx is called the *uncertainty in* x, introduced previously in Section 2.7.

Next, we calculate the expectation of the momentum for a particle in the state ψ, (3.37).

$$\langle p \rangle = \int_{-\infty}^{\infty} \psi^* \hat{p} \psi \, dx = \int_{-\infty}^{\infty} \psi^* \left(-i\hbar \frac{\partial}{\partial x} \right) \psi \, dx \tag{3.44}$$

$$= A^2 a \int_{-\infty}^{\infty} \left(p_0 + \frac{i\hbar}{2a} \eta \right) e^{-\eta^2/2} \, d\eta = p_0 \left(A^2 a \int_{-\infty}^{\infty} e^{-\eta^2/2} \, d\eta \right)$$

$$= p_0$$

It follows that the parameter p_0 which appears in the state function ψ is the average value of p. In any given measurement of p, any of a continuum of values can be obtained. Only in the event that ψ is an eigenfunction of $\hat{p}$ would measurement of p yield one definite value (i.e., the eigenvalue corresponding to the said eigenfunction).

PROBLEMS

3.10 For the state ψ, given by (3.37), show that

$$(\Delta x)^2 = a^2$$

Argue the consistency of this conclusion with the change in shape that $|\psi|^2$ suffers with a change in the parameter a.

3.11 Calculate the uncertainty Δp for a particle in the state ψ given by (3.37). Do you find your answer to be consistent with the uncertainty principle? (In this problem one must calculate $\langle \hat{p}^2 \rangle$. The operator $\hat{p}^2 = -\hbar^2 \, \partial^2/\partial x^2$.)

3.12 Let s be the number of spots shown by a die thrown at random.

(a) Calculate $\langle s \rangle$.

(b) Calculate Δs.

3.13 The number of hairs (N_l) on a certain rare species can only be the number 2^l ($l = 0, 1, 2, \ldots$). The probability of finding such an animal with 2^l hairs is $e^{-1}/l!$ What is the expectation, $\langle N \rangle$? What is ΔN?

\- Note: eqt$^{\underline{n}}$(3.45) implies any quantum system $\boxed{\text{in}}$ physics

observable space $\boxed{\text{in}}$ a containing space which is in intrensic evolution to ever reveal the physics which is now the space in which observation occurs.

* So when $V(\underline{r}) \to \hat{H}(\underline{r})$ does not imply that the system now does not belong to physics, and hence it is under the intrensic evolution provided by what is called the (time) i.e our system is under the action of a free fall in "the evolution which is time", hence the separation in eqt$^{\underline{n}}$(3.47).

* When $V(\underline{r},t)$ it is under the action of two evolutions:

$\boxed{1}$ One is provided by the fact that system belongs to physis which implies that it is under the free evolution of physics, "in terms of time".

$\boxed{2}$ The other, the system is containd under the constraining action provided by the evolution of the space $V(\underline{r},t)$.

* Eqt$^{\underline{n}}$ (3.47) implies that ψ (system space) is independent of any other space i.e V of the same evolution (time). Hence $\hat{H} = \hat{H}(\underline{r})$

=> "Space provided by $\underline{r}$" and "evolution space provided by t" are independent and hence can be convoluted i.e two spaces acting together $\underline{r}$ and t.

$\underline{1}$ ψ is a representative of the state of the ensemble at time (t) $\to$ as the components φ_n contributing to $\psi = \sum_{\forall n} b_n \varphi_n$ differs $\to$ $\langle x \rangle$ differs $\to$ once $\langle x \rangle = x_0$, and another time is $\langle x \rangle = x_0'$.

What is implied by an eigenstate, eigenfunction and State function?

(1) State function Ψ is not necessarily an eigenstate to any $\hat{A}$. (Ψ is an eigenf$^{\underline{n}}$ of $\hat{H}$ only and hence satisfies $\hat{A}\varphi = a\varphi$ when $\hat{A} \equiv \hat{H}$ only and therefore we can say that φ is Ψ revealing all the eigenstates φ_E of the $\hat{H}$) $\equiv$ Postulate (iv)

(2) φ is an eigenfunction to any $\hat{A}$, and when $\hat{A} \equiv \hat{H}$ we can replace φ by Ψ.

(3) φ_a is any of the revealed solutions resulting from solving the eigenvalue eq^{n} $\hat{A}\varphi = a\varphi$, hence φ_a is an eigenf$^{\underline{n}}$ as well.

* (4) The symbole Ψ is given to any time dependent state function as represented by a linear combination of the eigenstates of the operator $\hat{A} \Rightarrow \Psi(x,t) = \sum_{\forall a} b(t)\,\varphi_a$

i.e The A space is spanned by its basis eigenstates φ_a.

It is not necessarily that $\hat{A} \equiv \hat{H}$

$\Rightarrow \Psi(x,t)$ is a State function in the $\hat{A}$ Space.

This is a consequence of the Superposition principle.

3.4 TIME DEVELOPMENT OF THE STATE FUNCTION

Postulate IV

The fourth postulate of quantum mechanics specifies the time development of the state function $\psi(\mathbf{r}, t)$: the state function for a system (e.g., a single particle) develops in time according to the equation

a particular case in which the space of evolution is time (t).

$\forall t$, even if $\nexists$ measurment to A of $\hat{A}$

$$i\hbar \frac{\partial}{\partial t} \psi(\mathbf{r}, t) = \hat{H}\psi(\mathbf{r}, t) \tag{3.45}$$

This equation is called the *time-dependent Schrödinger* equation.[1] The operator $\hat{H}$ is the Hamiltonian operator. For a single particle of mass m, in a potential field $V(\mathbf{r})$, it is given by (3.12). If $\hat{H}$ is assumed to be independent of time, we may write

$$\hat{H} = \hat{H}(\mathbf{r}) \tag{3.46}$$

Under these circumstances, one is able to construct a solution to the time-dependent Schrödinger equation through the technique of separation of variables. We assume a solution of the form

$$\psi(\mathbf{r}, t) = \varphi(\mathbf{r})T(t) \tag{3.47}$$

Substitution into (3.45) gives

$$i\hbar \frac{T_t}{T} = \frac{\hat{H}\varphi}{\varphi} \tag{3.48}$$

The subscript t denotes differentiation with respect to t. Equation (3.48) is such that the left-hand side is a function of t only, while the right-hand side is a function of $\mathbf{r}$ only. Such an equation can be satisfied only if both sides are equal to the same constant, call it E (we do not yet know that E is the energy).

$$\hat{H}\varphi(\mathbf{r}) = E\varphi(\mathbf{r}) \tag{3.49}$$

$$\left(\frac{\partial}{\partial t} + \frac{iE}{\hbar}\right)T(t) = 0 \tag{3.50}$$

The first of these equations is the time-independent Schrödinger equation (3.13). This identification serves to label E, in (3.49), the energy of the system. That is, E, as it appears in this equation, is an eigenvalue of $\hat{H}$. But the eigenvalues of $\hat{H}$ are the allowed energies a system may assume, and we again conclude that E is the energy of the system.

---

[1] A formulation of the Schrödinger equation that has its origin in the classical principle of least action has been offered by R. P. Feynman, *Rev. Mod. Phys.* 60, 367 (1948). An elementary description of this derivation may be found in S. Borowitz, *Quantum Mechanics*, W. A. Benjamin, New York, 1967.

3 The second equation (3.50) is simply solved to give the oscillating form

$$T(t) = A \exp\left(-\frac{iEt}{\hbar}\right) \tag{3.51}$$

Suppose that we solve the time-independent Schrödinger equation and obtain the eigenfunctions and eigenvalues

$$\hat{H}\varphi_n = E_n\varphi_n \tag{3.52}$$

For each such eigensolution, there is a corresponding eigensolution to the time-dependent Schrödinger equation

$$\psi_n(\mathbf{r}, t) = A\varphi_n(\mathbf{r}) \exp\left(-\frac{iE_n t}{\hbar}\right) \tag{3.53}$$

† 1 In equations (3.52) and (3.53) the index n denotes the set of integers $n = 1, 2, \ldots$. This notation is appropriate to the case where solution to the time-independent Schrödinger equation gives a discrete set of eigenfunctions, $\{\varphi_n\}$. Such is the case for 1. problems that pertain to a finite system, such as a particle confined to a finite domain of space. We will encounter this property in Chapter 4 when we solve the problem of a bead constrained to move on a straight wire strung between two impenetrable walls.

2 In the one-dimensional free-particle case treated in Section 3.2, one obtains a continuum of eigenfunctions $\varphi_k(x)$ and, correspondingly, a continuum of eigenvalues, E_k. To repeat, these values are

$$\hat{H}\varphi_k = E_k\varphi_k \tag{3.54}$$

$$\varphi_k = A \exp(ikx), \qquad E_k = \frac{\hbar^2 k^2}{2m} \tag{3.55}$$

2. For each such time-independent solution, there is a solution to the time-dependent Schrödinger equation

$$\psi_k(x, t) = Ae^{i(kx - \omega t)} \tag{3.56}$$

where we have labeled

$$\hbar\omega = E_k \tag{3.57}$$

2 The structure of the solution (3.56) is characteristic of a propagating wave. More generally, any function of x and t of the form

$$f(x, t) = f(x - vt) \tag{3.58}$$

represents a wave propagating in the positive x direction with velocity v. To see this, we note the following property of f:

$$f(x + v\,\Delta t, t + \Delta t) = f(x, t) \tag{3.59}$$

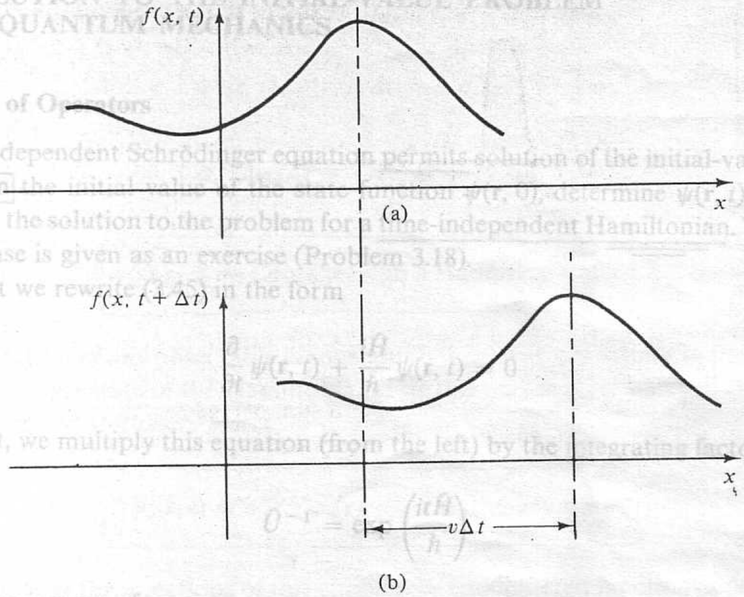


FIGURE 3.3 **Propagating wave, $f(x, t) = f(x - vt)$: (a) at time t; (b) at time $t + \Delta t$.**

At any given instant t, one may plot the x dependence of f (Fig. 3.3). If t increases to $t + \Delta t$, this curve is displaced to the right (as a rigid body) by the amount $v\,\Delta t$. We conclude from these arguments that the disturbance f (3.58) propagates with the wave speed v.

Now let us return to the free-particle eigenstate, (3.56), and rewrite it in the form

$$\psi_k(x, t) = A \exp\left[ik\left(x - \frac{\omega}{k}t\right)\right] \tag{3.60}$$

Comparison with the waveform (3.58) indicates that (1) ψ_k is a propagating wave (moving to the right), and (2) the speed of this wave is

$$v = \frac{\omega}{k} = \frac{\hbar\omega}{\hbar k} = \frac{p^2/2m}{p} = \frac{p}{2m} = \frac{v_{CL}}{2} \tag{3.61}$$

The velocity v_{CL} represents the classical velocity of a particle of mass m and momentum p. Thus we find that the wave speed of the state function of a particle with well-defined momentum, $p = \hbar k$, is half the classical speed, $v_{CL} = p/m$.

2 This discrepancy is due to the following fact. Suppose that we calculate the probability density corresponding to the state given in (3.56). We obtain the result that it is uniformly probable to find the particle anywhere along the x axis. This is not a

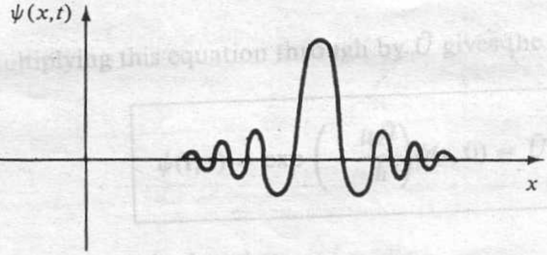


FIGURE 3.4 Wave packet at a given instant of time t.

3 typical classical property of a particle. The state function that better represents a classical (localized) particle is a wave packet. The shape of such a function is sketched † in Fig. 3.4. Such a state may be constructed as a sum of eigenstates of the form given in (3.56) (a Fourier series). The velocity with which the packet moves is called the *group velocity*,[1]

$$v_g = \frac{\partial \omega}{\partial k} \tag{3.62}$$

3· For a wave packet composed of free-particle eigenstates, v_g takes the value

$$\begin{aligned} v_g &= \frac{\partial \hbar\omega}{\hbar\,\partial k} = \frac{\partial(\hbar^2 k^2/2m)}{\hbar\,\partial k} = \frac{\hbar k}{m} = \frac{p}{m} \\ &= v_{CL} \end{aligned} \tag{3.63}$$

The value of k that enters the formula for v_g is the value about which there is a superabundance of ψ_k component waves. These topics will be more fully developed in Chapter 4. For the moment we are concerned only with the identification given in (3.63).

PROBLEMS

3.14 Describe the evolution in time of the following wavefunctions:

$$\begin{aligned} \psi_1 &= A \sin \omega t \cos k(x + ct) \\ \psi_2 &= A \sin (10^{-5} kx) \cos k(x - ct) \\ \psi_3 &= A \cos k(x - ct) \sin [10^{-5} k(x - ct)] \end{aligned}$$

3.15 What is the expectation of momentum $\langle p \rangle$ for a particle in the state

$$\psi(x, t) = Ae^{-(x/a)^2} e^{-i\omega t} \sin kx?$$

---

[1] The concepts of phase and group velocities are returned to in Section 6.1.

3.5 SOLUTION TO THE INITIAL-VALUE PROBLEM IN QUANTUM MECHANICS

Functions of Operators

The time-dependent Schrödinger equation permits solution of the initial-value problem: $\boxed{\text{given}}$ the initial value of the state function $\psi(\mathbf{r}, 0)$, determine $\psi(\mathbf{r}, t)$. We will formulate the solution to the problem for a time-independent Hamiltonian. The more general case is given as an exercise (Problem 3.18).

First we rewrite (3.45) in the form

$$\frac{\partial}{\partial t}\psi(\mathbf{r}, t) + \frac{i\hat{H}}{\hbar}\psi(\mathbf{r}, t) = 0 \tag{3.64}$$

Next, we multiply this equation (from the left) by the integrating factor $\hat{U}^{-1}$

$$\hat{U}^{-1} = \exp\left(\frac{it\hat{H}}{\hbar}\right) \tag{3.65}$$

which is the inverse of

$$\hat{U} \equiv \exp\left(-\frac{it\hat{H}}{\hbar}\right) \tag{3.66}$$

2 This function of the operator, $\hat{H}$, is itself an operator. It is defined in terms of its Taylor series expansion.

$$\hat{U}^{-1} = \exp\left(\frac{it\hat{H}}{\hbar}\right) = 1 + \frac{it\hat{H}}{\hbar} + \frac{1}{2!}\left(\frac{it\hat{H}}{\hbar}\right)^2 + \cdots \tag{3.67}$$

More generally for any operator $\hat{A}$, the function operator $f(\hat{A})$ is defined in terms of a series in powers of $\hat{A}$. A few examples are provided in the problems.

3 Let us return to the problem under discussion. Multiplying the time-dependent Schrödinger equation through by the integrating factor (3.65), one obtains the equation

$$\frac{\partial}{\partial t}\left[\exp\left(\frac{it\hat{H}}{\hbar}\right)\psi(\mathbf{r}, t)\right] = 0 \tag{3.68}$$

Integrating over the time interval $(0, t)$ gives

$$\exp\left(\frac{it\hat{H}}{\hbar}\right)\psi(\mathbf{r}, t) - \psi(\mathbf{r}, 0) = 0 \tag{3.69}$$

3 Multiplying this equation through by $\hat{U}$ gives the desired result:

$$\boxed{\psi(\mathbf{r}, t) = \exp\left(-\frac{it\hat{H}}{\hbar}\right)\psi(\mathbf{r}, 0) = \hat{U}\psi(\mathbf{r}, 0)} \tag{3.70}$$

Here we have used the fact that

$$\hat{U}\hat{U}^{-1} = \exp\left(-\frac{it\hat{H}}{\hbar}\right)\exp\left(\frac{it\hat{H}}{\hbar}\right) = \hat{I} \tag{3.71}$$

where $\hat{I}$ is the identity operator.

† 1 Suppose that in solution (3.70) we choose the initial state to be an eigenstate of $\hat{H}$. Call it φ_n, so that

$$\begin{aligned} \psi_n(\mathbf{r}, 0) &= \varphi_n(\mathbf{r}) \\ \hat{H}\varphi_n &= E_n\varphi_n \end{aligned} \tag{3.72}$$

1 By virtue of the theorem presented in Problem 3.16,

$$\begin{aligned} \psi_n(\mathbf{r}, t) = \exp\left(-\frac{it\hat{H}}{\hbar}\right)\varphi_n &= \exp\left(-\frac{iE_n t}{\hbar}\right)\varphi_n \\ &= e^{-i\omega_n t}\varphi_n(\mathbf{r}) \\ \hbar\omega_n &= E_n \end{aligned} \tag{3.73}$$

This is the solution of the time-dependent Schrödinger equation, derived in Section 3.4 by the technique of separation of variables. The solution given in (3.70) is more general. It exhibits the development of an arbitrary initial state $\psi(\mathbf{r}, 0)$ in time. It will be used extensively in the chapters to follow, where the student will gain a more workable understanding of the equation. 2

2 As a final topic of discussion in this chapter we note the following. Suppose that a system is in an eigenstate of the Hamiltonian at $t = 0$, described by (3.72). At this (initial) time the expectation of an observable A is

$$\langle A \rangle_{t=0} = \int \psi^*(\mathbf{r}, 0)\hat{A}\psi(\mathbf{r}, 0)\, d\mathbf{r} = \int \varphi_n{}^*\hat{A}\varphi_n\, d\mathbf{r} \tag{3.74}$$

1 What is $\langle A \rangle$ at a later time, $t > 0$? The state of the system at $t > 0$ is given by (3.73):

$$\psi_n(\mathbf{r}, t) = e^{i\omega_n t}\varphi_n(\mathbf{r}) \tag{3.75}$$

so that at $t > 0$ (assuming that $\partial \hat{A}/\partial t = 0$),

$$\langle A \rangle_t = \int \psi^*(\mathbf{r}, t)\hat{A}\psi(\mathbf{r}, t)\, d\mathbf{r} = e^{+i\omega_n t} e^{-i\omega_n t} \int \varphi_n{}^* \hat{A}\varphi_n\, d\mathbf{r}$$

$$= \int \varphi_n{}^* \hat{A}\varphi_n\, d\mathbf{r} = \langle A \rangle_{t=0} \tag{3.76}$$

$$\boxed{\langle A \rangle_{t>0} = \langle A \rangle_{t=0} \quad \text{in a stationary state}}$$

+2 The expectation of *any* observable is constant in time, if at any instant in time the system is in an eigenstate of the Hamiltonian. For this reason eigenstates of the Hamiltonian are called *stationary states.*

$$\boxed{\psi_n(\mathbf{r}, t) = e^{-i\omega_n t}\varphi_n(\mathbf{r}) \qquad \text{a stationary state}} \tag{3.77}$$

3 In the first three sections of this chapter we encountered functions relevant to a system which are eigenfunctions of operators corresponding to observable properties of that same system. In what sense are these eigenfunctions related to the *state function* of the system? From postulate II we know that ideal measurement of A leaves the system in the eigenstate of $\hat{A}$ corresponding to the value of A that was found in 3. measurement. Thus, the state function of the system immediately after measurement is this same eigenstate of $\hat{A}$. The state function then evolves in time according to (3.70).

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PROBLEMS

3.16 Let the eigenfunctions and eigenvalues of an operator $\hat{A}$ be $\{\varphi_n\}$ and $\{a_n\}$, respectively, so that

$$\hat{A}\varphi_n = a_n \varphi_n$$

Let the function $f(x)$ have the expansion

$$f(x) = \sum_{l=0}^{\infty} b_l x^l$$

Show that φ_n is an eigenfunction of $f(\hat{A})$ with eigenvalue $f(a_n)$. That is,

$$f(\hat{A})\varphi_n = f(a_n)\varphi_n$$

3.17 If $\hat{p}$ is the momentum operator in the x direction, and $f(x)$ is an arbitrary "well-behaved" function, show that

$$\exp\left(\frac{i\zeta\hat{p}}{\hbar}\right) f(x) = f(x+\zeta)$$

The constant ζ represents a small displacement. In this problem the student must demonstrate that the left-hand side of the equation above is the Taylor series expansion of the right-hand side about $\zeta = 0$.

3.18 If $\hat{H}$ is an explicit function of time, show that the solution to the initial-value problem (by direct differentiation) is

$$\psi(\mathbf{r}, t) = \exp\left[-\frac{i}{\hbar}\int_0^t dt'\hat{H}(t')\right]\psi(\mathbf{r}, 0)$$

You may assume that $\hat{H}(t)\hat{H}(t') = \hat{H}(t')\hat{H}(t)$.

3.19. What is the effect of operating on an arbitrary function $f(x)$ with the following two operators?

(a) $\hat{O}_1 \equiv (\partial^2/\partial x^2) - 1 + \sin^2(\partial^3/\partial x^3) + \cos^2(\partial^3/\partial x^3)$.

(b) $\hat{O}_2 \equiv \cos(2\partial/\partial x) + 2\sin^2(\partial/\partial x) + \int_a^b dx$.

3.20 (a) The time-dependent Schrödinger equation is of the form

$$a\frac{\partial\psi}{\partial t} = \hat{H}\psi$$

Consider that a is an unspecified constant. Show that this equation has the following property. Let $\hat{H}$ be the Hamiltonian of a system composed of two independent parts, so that

$$\hat{H}(x_1, x_2) = \hat{H}_1(x_1) + \hat{H}_2(x_2)$$

and let the stationary states of system 1 be $\psi_1(x_1, t)$ and those of system 2 be $\psi_2(x_2, t)$. Then the stationary states of the composite system are

$$\psi(x_1, x_2) = \psi_1(x_1, t)\psi_2(x_2, t) \qquad \sim (3.47)$$

That is, show that this product form is a solution to the preceding equation for the given composite Hamiltonian.

Such a system might be two beads that are invisible to each other and move on the same straight wire. The coordinate of bead 1 is x_1 and the coordinate of bead 2 is x_2.

(b) Show that this property is not obeyed by a wave equation that is second order in time, such as

$$a^2\frac{\partial^2\psi}{\partial t^2} = \hat{H}\psi$$

(c) Arguing from the Born postulate, show that the wavefunction for a system composed of two independent components must be in the preceding product form, thereby disqualifying the wave equation in part (b) as a valid equation of motion for the wavefunction ψ.

(3.24). $a\frac{\partial \psi}{\partial t} = \hat{H}\psi$ → the integrating factor is

1. $\exp(-\frac{1}{a} t \hat{H})$ if $\hat{H} \equiv \hat{H}(\underline{r})$

$\Rightarrow \psi(\underline{r},t) = \exp(\frac{1}{a} t \hat{H})\, \psi(\underline{r},0)$.

2. If $\hat{H} = \hat{H}(\underline{r},t) \Rightarrow$ the integrating factor is

$\exp\left(-\frac{1}{a}\int_0^t dt' \hat{H}(t')\right) \Rightarrow$

$\psi(\underline{r},t) = \exp\left(\frac{1}{a}\int^t dt' \hat{H}(t')\right) \psi(\underline{r},0)$

3. The two System will be visible to each other only when there is a relative Potential in between s.t. One can See the Presence of the other through the Potential produced by its presence. But $\hat{H}_1 = \hat{H}_1(x_1)$, $\hat{H}_2 = \hat{H}_2(x_2)$ by extrapolating the analogy between [$\hat{H} = \hat{H}(\underline{r}) \rightarrow$ $\psi(x,y,z,t) = \Phi(\underline{r})\, T(t) = \exp(-\frac{i}{\hbar} t \hat{H})\, \psi(\underline{r},0)$]

4. Here we do: $\hat{H} \equiv \hat{H}(\underline{r}) \equiv \hat{H}(x_1; x_2) = \hat{H}(x_1) + \hat{H}(x_2)$

$\rightarrow \psi((x_1;x_2)\, t)$ is Solved by the method of Separation of variables two times 1st (x_1,t), 2nd (x_2,t)

$\psi((x_1;x_2),t) = \psi_1(x_1,t)\, \psi_2(x_2,t) = \Phi(x_1)\, T_1(t)\, \Phi_2(x_2)\, T_2(t)$

$= \exp(-\frac{i}{\hbar} t \hat{H})\, \psi((x_1;x_2),0) = \exp(-\frac{i}{\hbar} t [H_1 + H_2])\, \psi((x_1;x_2),0)$

$= \left(\exp(-\frac{i}{\hbar} t H_1)\, \psi(x_1,0)\right)\left(\exp(-\frac{i}{\hbar} t \hat{H}_2)\, \psi(x_2,0)\right)$

(3.18) $\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\underline{r},t)\right] \equiv \hat{H}(\underline{r},t) \equiv \hat{H}$, $\hat{H}\psi(\underline{r},t) = i\hbar\frac{\partial}{\partial t}\psi(\underline{r},t)$ $\boxed{I}$

1 By looking back to (3.70) we notice when $\hat{H}(r) = \hat{H}$ the integrating factor is $\exp\left(\frac{i}{\hbar}\,t\,\hat{H}(r)\right)$ to $\boxed{I}$

2 When $\hat{H}(r,t) \equiv \hat{H}$ the integrating factor is

$$\exp\left(\frac{i}{\hbar}\int_0^t dt'\,\hat{H}(\underline{r},t')\right) \text{ to } \boxed{I}$$

* Did you notice the similarity the integrating factors in the two cases shear.

3 If $\psi(\underline{r},t) = \exp\left(-\frac{i}{\hbar}\int_0^t dt'\,\hat{H}(r,t')\right)\psi(\underline{r},0)$ (III) is to be a solution to $\boxed{I}$ → it solves $\boxed{I}$

3. Taking the derivative to both sides w.r to t →

$$\frac{\partial}{\partial t}\psi(\underline{r},t) = \frac{\partial}{\partial t}\left[e^{(\ )}\psi(\underline{r},0)\right] = \frac{\partial}{\partial t}e^{(\ )}\psi(\underline{r},0) + \cancel{e^{(\ )}\frac{\partial}{\partial t}\psi(\underline{r},0)}$$

$$= \frac{\partial}{\partial t}\left[-\frac{i}{\hbar}\int_0^t dt'\,\hat{H}(t')\right]\left[e^{(\ )}\psi(\underline{r},0)\right] =$$

$$-\frac{i}{\hbar}\frac{\partial}{\partial t}\left(\int_0^t dt'\,\hat{H}(t')\right)\psi(\underline{r},t) = \left[-\frac{i}{\hbar}\hat{H}\,\psi(\underline{r},t) = \frac{\partial}{\partial t}\psi(\underline{r},t)\right]$$

$$\Rightarrow \hat{H}(\underline{r},t)\Big|_{t'=t} = \hat{H}(\underline{r},t) = \hat{H} \Rightarrow$$

$$\hat{H}\psi(\underline{r},t) = i\hbar\frac{\partial}{\partial t}\psi(\underline{r},t)\Big|_{t'=t} \equiv \boxed{I}$$

4 ⇒ If we take the running variable for the time as t' ⇒

$$\hat{H}(\underline{r},t')\Big|_{t'=t} = \hat{H}(\underline{r},t) = \hat{H}(\underline{r}),\ t = \text{Constant}$$

but t or t' are dummy variables ⇒ we can assume that

$$\text{if } \int_0^t dt'\,\hat{H}(\underline{r},t') = \hat{H}(\underline{r},t')\Big|_{t'=t} = \hat{H}(\underline{r}) \rightarrow$$

$$\hat{H}(\underline{r},t)\int_0^t dt'\,\hat{H}(\underline{r},t') = \int_0^{t}\overset{t'=0}{dt'}\,\hat{H}(\underline{r},t)\,\hat{H}(\underline{r},t') = \int^t dt'\,\hat{H}(t')\,\hat{H}(t)$$

because the parameter t in $\hat{H}(t)$ is constant → $\hat{H}^{\circ}(t) = \hat{H}(\underline{r})$.

$$a\frac{\partial^2\Psi}{\partial t^2} = \hat{H}\Psi \quad , \Psi = \Psi_1(x_1,t)\,\Psi_2(x_2,t)$$

$$= (\hat{H}_1 + \hat{H}_2)\Psi$$

$$a\frac{\partial^2\Psi_1}{\partial t^2}\Psi_2 + a\Psi_1\frac{\partial^2\Psi_2}{\partial t^2} = \Psi_2\hat{H}_1\Psi_1 + \Psi_1\hat{H}\Psi_2$$

$$a\frac{\partial}{\partial t}\left(a\frac{\partial}{\partial t}\Psi\right) = \hat{H}\Psi \rightarrow$$

since when $\boxed{a\frac{\partial}{\partial t}\Psi = \hat{H}\Psi}$ $\boxed{\Psi = \Psi_1\Psi_2 \text{ is a solution}}$

$$\rightarrow a\frac{\partial}{\partial t} \quad \boxed{\Psi(r,t) = \Phi(r)T(t)}$$

$$\rightarrow \frac{a\frac{\partial}{\partial t}T}{T} = \frac{H\Phi}{\Phi} = E$$

$$\frac{aT_1\frac{\partial T_2}{\partial t} + aT_2\frac{\partial T_1}{\partial t}}{T_1\,T_2} = \frac{\Phi_2 H_1\Phi_1 + \Phi_1 H_2\Phi_2}{\Phi_1\,\Phi_2}$$

$$= E_1 + E_2$$

$$\hat{H} = (H_1 + H_2)\Phi = (E_1 + E_2)\Phi$$

$$a\frac{\partial}{\partial t}T = (E_1 + E_2)T \rightarrow$$

$$\boxed{T = ae^{\left(\frac{E_1+E_2}{a}\right)t}} = ae^{\frac{E_1}{a}t}e^{\frac{E_2 t}{a}}$$

$$\boxed{\Psi_n(x_1;x_2,t) = \left(ae^{\left(\frac{E_1+E_2}{a}\right)t}\right)(\Phi)}$$

$$\rightarrow \left(a\frac{\partial}{\partial t}\right)\underline{\left(a\frac{\partial}{\partial t}\right)\Psi} = \hat{H}\Psi$$

$$a\frac{\partial}{\partial t}(\hat{H}\Psi) = (\hat{H}\Psi)$$

$$a\frac{\partial}{\partial t}$$

$$a\frac{\partial}{\partial t}(T\hat{H}\phi) = T\hat{H}\phi$$

$$= a\left(\frac{E_1+E_2}{a}\right)T\hat{H}\phi + aT\boxed{\cancel{\frac{\partial}{\partial t}(\hat{H}\phi)}}$$

$$\Rightarrow \boxed{(E_1+E_2)\hat{H}\psi = \hat{H}\psi}$$

$$\Rightarrow \boxed{E_1+E_2=1}$$

which is a restrictive eqtn because it relates the energies of the two systems in such an unnecessary way when $H\psi$ do not restrict us in any way so no restrictions on the E_1 or E_2 why they emerge s.t. $\boxed{E_1+E_2=1}$

$$a\frac{\partial\psi}{\partial t} = \underline{\hat{H}\psi = E\psi} \Rightarrow$$

if $a\frac{\partial}{\partial t}(\hat{H}\psi) = \hat{H}\psi \rightarrow$

$$\boxed{a^2\frac{\partial^2}{\partial t^2}\psi = a\frac{\partial}{\partial t}(\hat{H}\psi) = aE\frac{\partial}{\partial t}\psi \atop E(\hat{H}\psi)}$$

$$\left(a\frac{\partial}{\partial t}\right)^2\psi = a\frac{\partial}{\partial t}(\hat{H}\psi) = \underline{E(\hat{H}\psi) \atop E^2\psi}$$

a^2

Answer (partial)

(c) If the two components are independent of each other, the joint probability density describing the state of the system is given by

$$P_{12} = P_1 P_2$$

This, in turn, guarantees that the probability density associated with component 1,

$$P_1(x_1) = \int P_{12}(x_1, x_2)\, dx_2$$

is independent of the form of $P_2(x_2)$ (and vice versa). The product form for P_{12} is guaranteed by the product structure for the wavefunction $\psi(x_1, x_2)$.

3.21 It is established in Problem 3.20 that for the joint probability for two independent systems to be consistently described by the time-dependent Schrödinger equation, this equation must be of the form

$$a\frac{\partial \psi}{\partial t} = \hat{H}\psi$$

where a is some number. Show that for this equation to imply wave motion, a must be complex. You may assume that $\hat{H}$ has only real eigenvalues.

Answer

Following development of the general solution (3.70), we find that the given equation implies the solution

$$\psi(\mathbf{r}, t) = \exp\left(\frac{t\hat{H}}{a}\right)\psi(\mathbf{r}, 0)$$

Since $\hat{H}$ has only real eigenvalues, the time dependence of $\psi(\mathbf{r}, t)$ is nonoscillating. It modulates $\psi(\mathbf{r}, 0)$ in time and does not give propagation. Thus, if a is real, ψ cannot represent a propagating wave. (*Note:* The fact that a is complex implies that ψ is complex. These last two problems illustrate the necessity of complex wavefunctions in quantum mechanics.)

Why Physics is Generated?

CHAPTER 4

PREPARATORY CONCEPTS. FUNCTION SPACES AND HERMITIAN OPERATORS

4.1 *Particle in a Box and Further Remarks on Normalization*
4.2 *The Bohr Correspondence Principle*
4.3 *Dirac Notation*
4.4 *Hilbert Space*
4.5 *Hermitian Operators*
4.6 *Properties of Hermitian Operators*

where our observation are
Why we observe ≡ teller ≡ how information is transfered

Having the physics generated, Hermitian operators are readily available of the elements of physics, i.e they need not be revealed.
To the observing element to know why the presence of A enables observation, he must derive it in the form of a mathematical structure. (Mind, Time, Space (generally)) and Physics (generated)
"Time is the reventer of the mathematical structure = Space"

In this and the following two chapters, we continue development of physical principles and mathematical groundwork important to quantum mechanical descriptions. Included in the present chapter are the notions of Hilbert space and Hermitian operators. First, we obtain wavefunctions relevant to a particle in a one-dimensional box. These, together with previously derived free-particle wavefunctions, then serve as simply understood references for subsequent descriptions of Hilbert space and Hermitian operators.

4.1 PARTICLE IN A BOX AND FURTHER REMARKS ON NORMALIZATION

In chapter 3 we solved the quantum mechanical free-particle problem. We recall that the free-particle Hamiltonian generates a continuous spectrum of eigenvalues, $\hbar^2 k^2/2m$, and eigenfunctions, $\varphi_k = A \exp(ikx)$, as given in (3.55).

The second one-dimensional problem we wish to treat is that of a point mass m, constrained to move on an infinitely thin, frictionless wire which is strung tightly between two impenetrable walls a distance L apart (see Fig. 4.1). The corresponding

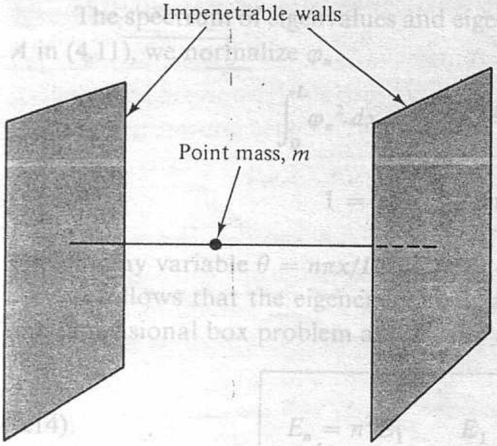


FIGURE 4.1 One-dimensional "box."

potential has the values

$$
\begin{aligned}
&V(x) = \infty \qquad (x \le 0, \quad x \ge L) \qquad &\text{(domain 1)}\\
&V(x) = 0 \qquad (0 < x < L) \qquad &\text{(domain 2)}
\end{aligned}
\tag{4.1}
$$

and is depicted in Fig. 4.2. This configuration is known as the *one-dimensional box*.[1]

The Hamiltonian for this problem is the following operator:

$$\hat{H}_1 = \frac{\hat{p}^2}{2m} + \infty = \infty \qquad (x \le 0, \quad x \ge L) \qquad \text{(domain 1)} \tag{4.2}$$

$$\hat{H}_2 = \frac{\hat{p}^2}{2m} \qquad (0 < x < L) \qquad \text{(domain 2)} \tag{4.3}$$

In domain 1 the time-independent Schrödinger equation gives $\varphi = 0$. For any finite eigenenergy E, in this domain the time-independent Schrödinger equation reads

$$\hat{H}_1 \varphi = E\varphi \tag{4.4}$$

Since φ and E are finite, the right-hand side is finite. Therefore, the left-hand side is finite and φ must vanish in this domain.

The fact that $\varphi = 0$ in domain 1 implies that there is zero probability that the particle is found there ($|\varphi|^2 = 0$). This is in agreement with the discussion in Chapter 1 on "forbidden domains." These, we recall, are domains where $E < V$. Certainly, this is the case in domain 1 for any finite energy E.

---

[1] A mathematically more accurate description of the one-dimensional box is: an infinitesimally thin, flat sheet of infinite extent and finite mass which moves between two walls of infinite extent. The two walls and sheet are all parallel and the velocity of the sheet is normal to the walls. Every point in space is then characterized by one coordinate, the normal displacement of the sheet from either of the walls.

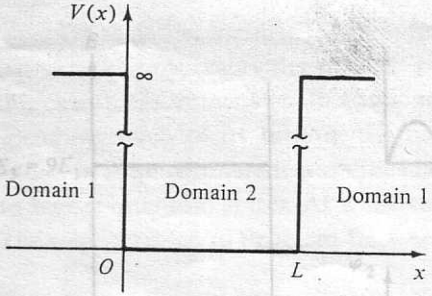


FIGURE 4.2 Potential corresponding to the one-dimensional box.

In domain 2 the time-independent Schrödinger equation is

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\varphi_n = E_n\varphi_n \tag{4.5}$$

The subscript n is in anticipation of a discrete spectrum of energies E_n and eigenfunctions φ_n.

Since φ_n is a continuous function, it must have the values

$$\varphi_n(0) = \varphi_n(L) = 0 \tag{4.6}$$

First we rewrite (4.5) in the form

$$\frac{\partial^2\varphi_n}{\partial x^2} + k_n{}^2\varphi_n = 0 \tag{4.7}$$

$$k_n{}^2 = \frac{2mE_n}{\hbar^2} \tag{4.8}$$

This is merely a change of variables from energy E_n to wavenumber k_n. The solution to (4.7) appears as

$$\varphi_n = A\sin k_n x + B\cos k_n x \tag{4.9}$$

The boundary conditions (4.6) give

$$B = 0 \tag{4.10}$$

$$A\sin k_n L = 0 \tag{4.11}$$

The second of these equations serves to determine the eigenvalues k_n.

$$k_n L = n\pi, \qquad n = 0, 1, 2, \ldots \tag{4.12}$$

a sequence

This is seen to be equivalent to the requirement that an integral number of half-wavelengths, $n(\lambda/2)$, fit into the width L.

The spectrum of eigenvalues and eigenfunctions is discrete. To find the constant A in (4.11), we normalize φ_n.

$$\int_0^L \varphi_n{}^2\,dx = 1 = A^2 \int_0^L \sin^2\left(\frac{n\pi x}{L}\right) dx \tag{4.13}$$

$$1 = \frac{A^2 L}{n\pi}\int_0^{n\pi} \sin^2\theta\,d\theta = \frac{A^2 L}{2}$$

The dummy variable $\theta = n\pi x/L$.

It follows that the eigenenergies E_n and normalized eigenfunctions φ_n for the one-dimensional box problem are

$$\boxed{E_n = n^2 E_1 \qquad E_1 = \frac{\hbar^2 k_1{}^2}{2m} = \frac{\hbar^2\pi^2}{2mL^2}} \tag{4.14}$$

$$\boxed{\varphi_n = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)} \tag{4.15}$$

The eigenstate corresponding to $n = 0$ is $\varphi = 0$. This, together with the solution in domain 1, gives $\varphi = 0$ over the whole x axis. There is zero probability of finding the particle anywhere. This is equivalent to the statement that the particle does not exist in the $n = 0$ state. Another argument that disallows the $n = 0$ state follows from the uncertainty principle. The energy corresponding to $n = 0$ is $E = 0$. Since the energy in domain 2 is entirely kinetic, this, in turn, implies that the particle is in a state of absolute rest ($\Delta p = 0$), an illegitimate state of affairs for a particle constrained to move in a finite domain.

The eigenenergies and eigenfunctions given by (4.14) and (4.15), together with the corresponding probability densities $|\varphi_n|^2$, are sketched in Fig. 4.3.

The Arbitrary Phase Factor

In concluding this section we note the following important fact. As described in Section 3.3, the wavefunction ψ gives information about a system through calculation of averages of observable properties of that system, according to the rule

$$\langle C\rangle = \int \psi^* \hat{C}\psi\,dx$$

This equation, as well as the normalization condition

$$\int \psi^*\psi\,dx = 1$$

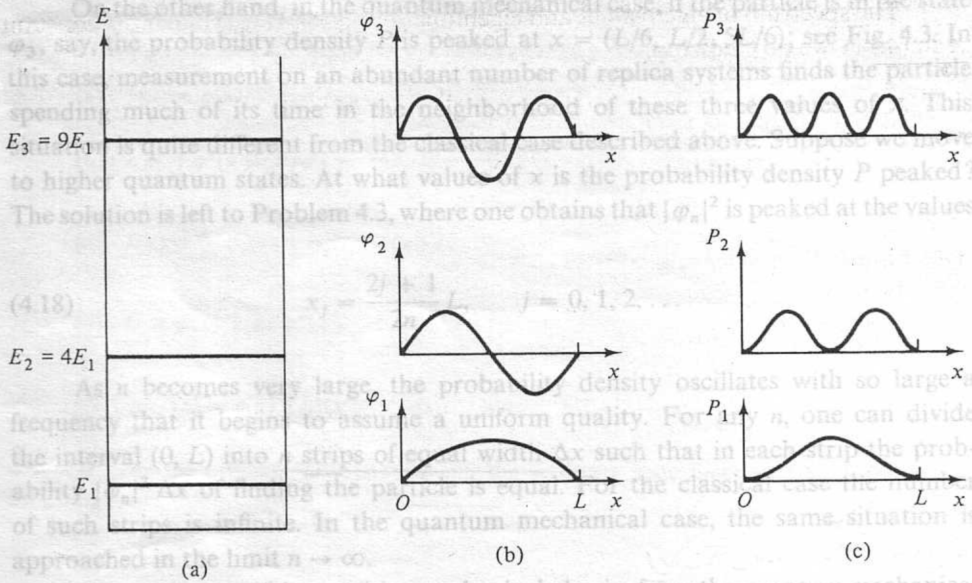


FIGURE 4.3 **(a) Eigenenergies for the one-dimensional box problem. (b) Eigenstates for the one-dimensional box problem:**

$$\varphi_n = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)$$

(c) Probability densities for the one-dimensional box problem:

$$P_n \equiv |\varphi_n|^2 = \frac{2}{L}\sin^2\left(\frac{n\pi x}{L}\right)$$

and therefore we can always say that ψ is Complex.

are invariant under the transformation $\psi \to e^{i\alpha}\psi$, where α is any real number. That is, a wavefunction is determined only to within a constant *phase factor* of the form $e^{i\alpha}$. Although associated with all wavefunctions, this arbitrary quality has no effect upon any physical results.[1]

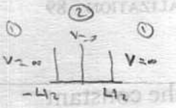
PROBLEMS

4.1 What are the eigenfunctions and eigenvalues for the one-dimensional box problem described above if the ends of the box are at $-L/2$ and $+L/2$?

4.2 For what values of the real angle θ will the constant $C = \frac{1}{2}(e^{i\theta} - 1)$ have no effect in calculations involving the modulus $|C\psi|$?

---

[1] On the other hand, component phase factors for a composite wavefunction such as that discussed in Section 2.5 do contribute to measurable effects, such as interference.



In Domain ① $\varphi(x) = 0 \quad \forall |x| \geq \frac{L}{2}$

In Domain2 ② $\hat{H}\varphi_n = E_n\varphi_n \Rightarrow -\frac{\hbar^2}{2m}\frac{\partial^2\varphi_n}{\partial x^2} = E_n\varphi_n$

* $\Rightarrow \frac{\partial^2\varphi_n}{\partial x^2} + \frac{2mE_n}{\hbar^2}\varphi_n = 0$ i.e $\varphi_{n_{xx}} + k^2\varphi_n = 0$

which has the general solution $\varphi_n = A\cos kx + B\sin kx$

* wanted k, E_k, φ_k, $\Rightarrow$ let us apply the Condition for the Continuity of φ_n

$\varphi(-\frac{L}{2}) = \varphi(\frac{L}{2}) = 0 \Rightarrow A\cos\frac{L}{2}k + B\sin\frac{L}{2}k = A\cos\frac{L}{2}k - B\sin\frac{L}{2}k = 0$

taking either $A=0$, or $B=0 \Rightarrow$ taking $\boxed{B=0} \Rightarrow$

$A\cos\frac{L}{2}k = 0 \Rightarrow \frac{L}{2}k = \frac{m}{2}\pi$, $m = 1, 3, 5, \ldots$

$m = n+1$, $n = 0, 2, 4, \ldots \Rightarrow k = \frac{m\pi}{L} \Rightarrow E_n = \frac{\hbar^2}{2m}\left(\frac{n+1}{L}\pi\right)^2$

* to obtain the Constant $A \Rightarrow$ let us apply the Normalization Conditions

$\int_{-L/2}^{L/2}\varphi^2\,dx = 1 \Rightarrow A^2\int_{-L/2}^{L/2}\cos^2 kx\,dx = 1$, $\cos 2\theta = 2\cos^2\theta - 1 \Rightarrow$

$A^2\int_{-L/2}^{L/2}\frac{\cos(2kx)+1}{2}\,dx = \frac{A^2}{4k}\int_{-kL}^{kL}\cos 2kx\,d(2kx) + \frac{A^2}{2}\times\frac{L}{x} = 1$

$2kx = X \Rightarrow \pm 2k\frac{L}{2} = X = m\theta$ $\quad \frac{A^2}{4k}\sin X\Big|_{-m\pi}^{m\pi} = \frac{A^2}{4k}2\sin m\pi = 0$

$kL = m\pi$, $1, 3, m\pi$ $\quad A^2 = 2/L \Rightarrow A = \sqrt{2/L}$

$\varphi_m = \sqrt{\frac{2}{L}}\cos\left(\frac{m\pi}{L}\right)x$, $m = 1, 3, 5, \ldots$ i.e m (odd) (1)

* If $A=0$, there is Corresponding solutions for m even $= 0, 2, 4, \ldots$

$\tilde{\varphi}_m = \sqrt{\frac{2}{L}}\sin\left(\frac{m\pi}{L}x\right)$ $m = 2, 4, 6, \ldots$ (even) (2)

4.2 THE BOHR CORRESPONDENCE PRINCIPLE

Let us now consider the *classical* motion of a particle in a one-dimensional box. As described previously, this configuration is effected by a bead sliding with no friction on a taut wire strung between two impenetrable walls a distance L apart. If the particle is given a velocity v, its motion (between collisions with the wall) is

$$x = x_0 + vt$$

Now suppose that the initial position x_0 is completely unknown. What is the probability $P\,dx$ of finding the particle in the interval x, $x + dx$, at a subsequent time? The answer is: the fraction of time dt/T it spends in this interval.

$1 \to T$

$\to dt$

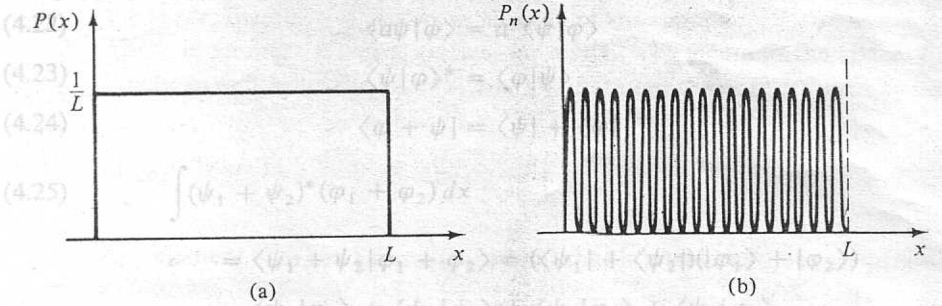
$$P\,dx = \frac{dt}{T} = \frac{v\,dt}{L} = \frac{dx}{L} \tag{4.16}$$

$v = \frac{L}{T}$

so that

$$P = \frac{1}{L} = \text{constant} \tag{4.17}$$

It is uniformly probable to find the particle at any position on the wire. If we make a large number of replicas of this one-dimensional system, measurement (at random times) of the coordinate x of the bead will find all values ($0 \leq x \leq L$) occurring equally often (Fig. 4.4).



(a) (b)

FIGURE 4.4 **(a) Classical probability density for the one-dimensional box. (b) Quantum mechanical probability density**

$$P_n = |\varphi_n|^2$$

for the one-dimensional box problem, for the case $n \gg 1$. The probability P_n vanishes $n + 1$ times in the interval $(0, L)$.

On the other hand, in the quantum mechanical case, if the particle is in the state φ_3, say, the probability density P is peaked at $x = (L/6, L/2, 5L/6)$; see Fig. 4.3. In this case, measurement on an abundant number of replica systems finds the particle spending much of its time in the neighborhood of these three values of x. This situation is quite different from the classical case described above. Suppose we move to higher quantum states. At what values of x is the probability density P peaked? The solution is left to Problem 4.3, where one obtains that $|\varphi_n|^2$ is peaked at the values

$$x_j = \frac{2j+1}{2n} L, \qquad j = 0, 1, 2, \ldots \tag{4.18}$$

2 As n becomes very large, the probability density oscillates with so large a frequency that it begins to assume a uniform quality. For any n, one can divide the interval $(0, L)$ into n strips of equal width Δx such that in each strip the probability $|\varphi_n|^2 \, \Delta x$ of finding the particle is equal. For the classical case the number of such strips is infinite. In the quantum mechanical case, the same situation is approached in the limit $n \to \infty$.

3 One encounters this transition to classical physics from the quantum mechanical domain in many problems. Bohr was the first to analyze this transition and offered the general rule that a quantum mechanical result must reduce to its classical counterpart in the classical domain. Since classical formulas do not contain $\hbar$, such a transition should be realized in the limit that $\hbar$ becomes small. For many problems this limit is attained in passing to high quantum numbers ($n \to \infty$). This rule is called the *Bohr correspondence principle.*

2 Classical physics includes the dynamics of macroscopic bodies. An aggregate of particles (e.g., a gas) obeys classical laws when the de Broglie wavelength, $\bar{\lambda}$, of a typical particle is small compared to all relevant lengths. For example, if the density of particles (number/cm^3) is n, the gas obeys classical statistics if $\lambda \ll n^{-1/3}$ (the mean distance between particles is $n^{-1/3}$). In the classical limit, fluctuations about the average become small and the probabilities indigenous to quantum mechanics reduce to certainties.

2 A rule of thumb in this area is that any quantum mechanical result that does not contain $\hbar$ is in essence a classical result. The first (fortuitous) example of this rule was Rutherford's classical calculation of the Coulomb cross section, relevant to the scattering of charged particles. The correct quantum mechanical calculation of this parameter is found not to contain $\hbar$. Rutherford's classical calculation yields the same result.

More examples of the correspondence principle will arise in the course of development of the text. Coulomb scattering is further described in Section 14.4.

(4.3) $\varphi_n = \sqrt{\frac{2}{L}} \sin(\frac{\pi n}{L} x) \Rightarrow P_n = |\varphi|^2 = \frac{2}{L} \sin^2(\frac{n\pi}{L} x)$

Since the sine function is max. or min. at $\frac{d}{dx} \sin(\frac{\pi n}{L} x) = 0$,

$0 \leq x \leq L \Rightarrow \frac{n\pi}{L} \cos(\frac{n\pi}{L} x) = 0, \rightarrow n \neq 0 \rightarrow$

$\frac{n\pi}{L} x = m\frac{\pi}{2}$, m odd $\rightarrow x_m = \frac{m}{2n} L = \frac{(2j+1)}{2n} L$

$x \leq L \rightarrow \frac{m}{2n} \leq 1 \overset{\text{when}}{\Rightarrow} m = 2j+1 \leq 2n, \ j = 0, 1, 2, \ldots$

$2j \leq 2n-1 \rightarrow j \leq n - \frac{1}{2}, \ n \in \mathbb{N}^+$

$* \text{ Since } j \in \mathbb{N}^+ \rightarrow n - \frac{1}{2} \notin \mathbb{N} \rightarrow j < n - \frac{1}{2} \rightarrow j = n-1$

which is the nearest integral value of $j < n - \frac{1}{2}, \rightarrow j = 0, 1, \ldots, n-1$.

PROBLEMS

4.3 For the one-dimensional box problem, show that $P = |\varphi_n|^2$ is maximum at the values $x = x_j$ given by

$$x_j = \frac{2j+1}{2n} L, \qquad j = 0, 1, 2, \ldots, n-1$$

4.3 DIRAC NOTATION

In this section we introduce a notation that proves to be an invaluable tool in calculation, called the *Dirac notation*. It gives a monogram to the integral of the product of two state functions, $\psi(x)$ and $\varphi(x)$, which appears as

$$\langle \psi | \varphi \rangle = \int_{-\infty}^{\infty} \psi^*(x)\varphi(x)\, dx \tag{4.19}$$

In Dirac notation, the integral on the right is written in the form shown on the left.

1 More generally, the integral operation $\langle \psi | \varphi \rangle$ denotes: (1) take the complex conjugate of the object in the first slot ($\psi \to \psi^*$) and then, (2) integrate the product
2 ($\psi^*\varphi$). This operation has the following simple properties. If a is any complex number and the functions ψ and φ are such that

$$\int_{-\infty}^{\infty} \psi^*\varphi\, dx < \infty \tag{4.20}$$

the following rules hold:

$$\langle \psi | a\varphi \rangle = a\langle \psi | \varphi \rangle \tag{4.21}$$

$$\langle a\psi | \varphi \rangle = a^*\langle \psi | \varphi \rangle \tag{4.22}$$

$$\langle \psi | \varphi \rangle^* = \langle \varphi | \psi \rangle \tag{4.23}$$

$$\langle \varphi + \psi | = \langle \psi | + \langle \varphi | \tag{4.24}$$

$$\int (\psi_1 + \psi_2)^*(\varphi_1 + \varphi_2)\, dx \tag{4.25}$$

$$= \langle \psi_1 + \psi_2 | \varphi_1 + \varphi_2 \rangle = (\langle \psi_1 | + \langle \psi_2 |)(|\varphi_1\rangle + |\varphi_2\rangle)$$

$$= \langle \psi_1 | \varphi_1 \rangle + \langle \psi_1 | \varphi_2 \rangle + \langle \psi_2 | \varphi_1 \rangle + \langle \psi_2 | \varphi_2 \rangle$$

3 The object $\langle \psi |$ (called a "bra vector") has an inevitable fate. Eventually, it is integrated in a product form with a ("ket vector") $|\varphi\rangle$, to form the "bra-ket," $\langle \psi | \varphi \rangle$.

Dirac notation is not complicated. The properties above tell the whole story. We move next to function spaces, where $\langle \varphi | \psi \rangle$ assumes a geometrical quality.

PROBLEMS

4.4 Write the following equations for the state vectors f, g, and so on, in Dirac notation.

(a) $f(x) = g(x)$.

(b) $c = \int g^*(x')h(x')\,dx'$.

(c) $f(x) = \sum_n \varphi_n(x) \int \varphi_n{}^*(x') f(x')\,dx'$.

(d) $\hat{O} \equiv \psi(x) \int dx' \varphi^*(x')$.

(e) $\dfrac{\partial}{\partial x} f(x) = h(x) \int h^*(x')g(x')\,dx'$.

4.5 Consider the operator $\hat{O} = |\varphi\rangle\langle\psi|$ and the arbitrary state function $f(x)$. Describe the following forms.

(a) $\langle f|\hat{O}$.
(b) $\hat{O}|f\rangle$.
(c) $\langle f|\hat{O}|f\rangle$.
(d) $\langle f|\hat{O}|\varphi\rangle$.

Answer (partial)

(a) $\langle f|\hat{O}$ is the bra vector $C\langle\psi|$, where the constant $C \equiv \langle f|\varphi\rangle = \int_{\infty}^{\infty} f^*\varphi\,dx$.

4.4 HILBERT SPACE

In this section we introduce the concept of a space of functions. Specifically we will deal with a Hilbert space. This serves the purpose of giving a geometrical quality to some of the abstract concepts of quantum mechanics.

We recall that in Cartesian 3-space a vector **V** is a set of three numbers, called components (V_x, V_y, V_z). Any vector in this space can be expanded in terms of the three unit vectors $\mathbf{e}_x$, $\mathbf{e}_y$, $\mathbf{e}_z$ (Fig. 4.5). Under such conditions one terms the triad $\mathbf{e}_x$, $\mathbf{e}_y$, $\mathbf{e}_z$, a *basis*.

(4.26) $$\mathbf{V} = \mathbf{e}_x V_x + \mathbf{e}_y V_y + \mathbf{e}_z V_z$$

The vectors $\mathbf{e}_x$, $\mathbf{e}_y$, $\mathbf{e}_z$ are said to *span* the vector space.

The inner ("dot") product of two vectors (**U** and **V**) in the space is defined as

(4.27) $$\mathbf{V}\cdot\mathbf{U} = V_x U_x + V_y U_y + V_z U_z$$

The length of the vector **V** is $\sqrt{\mathbf{V}\cdot\mathbf{V}}$.

(a) $|h\rangle = |g\rangle$, (b) $c = \langle g|h\rangle$,

(c) $|h\rangle = h(x) = \sum_n |\varphi_n\rangle\langle\varphi_n|h\rangle = (\sum |\varphi_n\rangle\langle\varphi_n|)|h\rangle = I|h\rangle = |h\rangle$

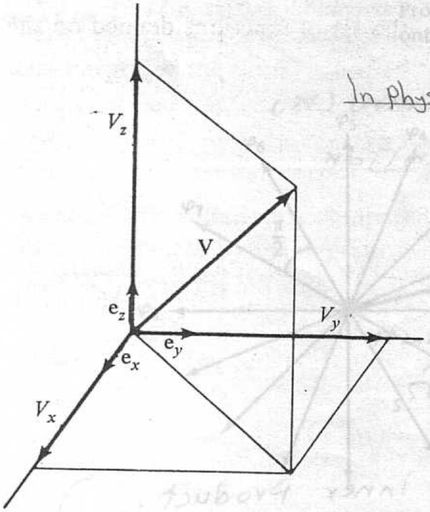
(d) $\hat{O} \equiv |\psi\rangle\langle\varphi|$, (e) $\frac{\partial}{\partial x}|h\rangle = |h\rangle\langle h|g\rangle = D|h\rangle$

5) (a) $\langle h|\varphi\rangle\langle\psi| = \langle\psi|\int h^*(x')\,\varphi(x')\,dx' = \langle h|\hat{O}$ bra vector

(b) $\hat{O}|h\rangle = |\varphi\rangle\langle\psi|h\rangle = |\varphi\rangle\int\psi^* h\,dx$ ket vector

(c) $\langle h|\hat{O}|h\rangle = \langle h|\varphi\rangle\langle\psi|h\rangle =$ Scalar

(d) $\langle h|\varphi\rangle\langle\psi|\varphi\rangle =$ (Scalar)



In physics , why ϕ_a is not observable w.r.t. Q?

≡ why ϕ_a is mathematical ?

FIGURE 4.5 Vector V in Cartesian 3-space and its components (V_x, V_y, V_z). The orthogonal triad $(\mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z)$ spans the space.

Why: Quantum Physics <=> Hilbert Space ?

A Hilbert space is much the same type of object. Its elements are functions instead of three-dimensional vectors. The similarity is so close that the functions are sometimes called vectors. A Hilbert space $\mathfrak{H}$ has the following properties.

1. The space is linear. A function space is linear under the following two conditions: (a) If a is a constant and φ is any element of the space, then $a\varphi$ is also an element of the space. (b) If φ and ψ are any two elements of the space, then $\varphi + \psi$ is also an element of the space.
2. There is an *inner product*, $\langle \psi | \varphi \rangle$, for any two elements in the space. For functions defined in the interval $a \leq x \leq b$ (in one dimension), we may take

$$\langle \varphi | \psi \rangle = \int_a^b \varphi^* \psi \, dx \tag{4.28}$$

3. Any element of $\mathfrak{H}$ has a norm ("length") that is related to the inner product as follows:

$$(\text{norm of } \varphi)^2 = \| \varphi \|^2 = \langle \varphi | \varphi \rangle \tag{4.29}$$

4. $\mathfrak{H}$ is complete. Every Cauchy sequence of functions in $\mathfrak{H}$ converges to an element of $\mathfrak{H}$. A Cauchy sequence $\{\varphi_n\}$ is such that $\| \varphi_n - \varphi_l \| \to 0$ as n and l approach infinity. (See Problem 4.24.) Loosely speaking, a Hilbert space contains all its limit points.

·2 An example of a Hilbert space is given by the set of functions defined on the interval $(0 \leq x \leq L)$ with finite norm

$$\boxed{\|\varphi\|^2 = \int_0^L \varphi^* \varphi \, dx < \infty \qquad \mathfrak{H}_1} \tag{4.30}$$

Another example is the space of functions commonly referred to by mathematicians as "L^2 space." This is the set of square-integrable functions defined on the whole x interval.

$$\boxed{\|\varphi\|^2 = \int_{-\infty}^{\infty} \varphi^* \varphi \, dx < \infty \qquad \mathfrak{H}_2} \tag{4.31}$$

1 Let us see how the preceding concept of inner product (4.28) is similar to the definition of the inner product between two finite-dimensional vectors (4.27). To see this we interpret the function $\varphi(x)$ as a vector with infinitely many components. These components are the values that φ assumes at each distinct value of its independent variable x. Just as the inner product between **U** and **V** is a sum over the products of parallel components, so is the inner product between φ and ψ a sum over parallel components. This sum is nothing but the integral of the product of φ and ψ. The reason we complex-conjugate the first "vector" is to ensure that the "length" (square root of the inner product between a "vector" φ and itself) of a vector φ is real.

Thus we see that Hilbert space is closely akin to a vector space. Mathematicians[1] call it that—an infinite-dimensional vector space (also: a complete, normed, linear vector space). Elements of this space have length and one can form an inner product between any two elements. The vector quality of Hilbert space can be pushed a bit further. We recall that if two vectors **U** and **V** in three-dimensional vector space are orthogonal to each other, their inner product vanishes. In a similar vein two vectors in Hilbert space, φ and ψ, are said to be orthogonal if

$$\langle \varphi | \psi \rangle = 0 \tag{4.32}$$

2 Furthermore, we recall that the three unit vectors $\mathbf{e}_x$, $\mathbf{e}_y$, and $\mathbf{e}_z$ "span" 3-space. Similarly, there is a set of vectors that "spans" Hilbert space. For instance, the Hilbert space whose elements all have the property given by (4.30) is spanned by the sequence of functions $\{\varphi_n\}$, which are the eigenfunctions of the Hamiltonian relevant

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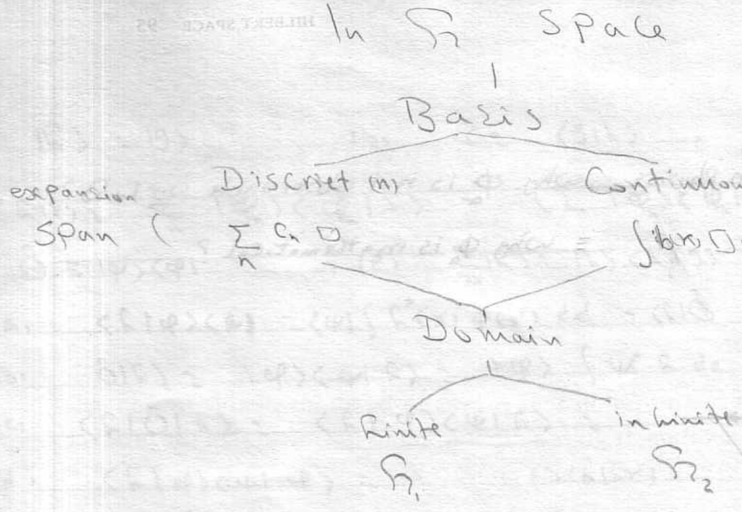
[1] A more mathematically accurate presentation of function spaces may be found in C. Goffman and G. Pedrick, *First Course in Functional Analysis*, Prentice-Hall, Englewood Cliffs, N.J., 1965. Another book in this area, but more directly related to quantum mechanics, is T. F. Jordan, *Linear Operators for Quantum Mechanics*, Wiley, New York, 1969.



[orthogonal, projection, inner product.
basis, span, expansion]

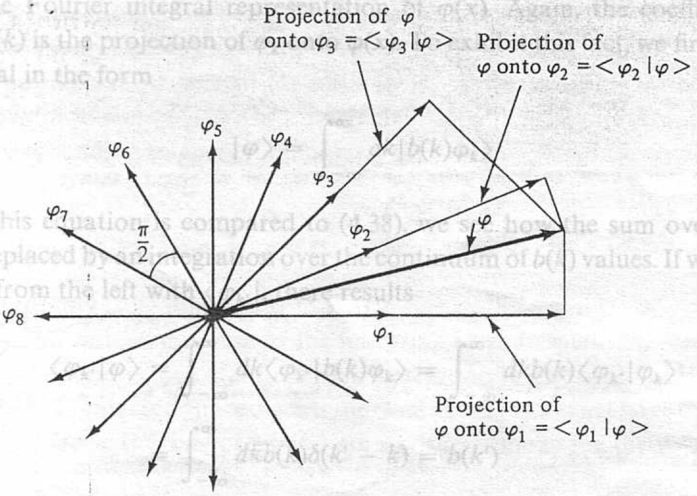

Projection of φ onto $\varphi_3 = \langle\varphi_3|\varphi\rangle$
Projection of φ onto $\varphi_2 = \langle\varphi_2|\varphi\rangle$
φ_5
φ_4
φ_6
φ_3
φ_7
φ
φ_2
$\frac{\pi}{2}$
φ_8
φ_1
Projection of φ onto $\varphi_1 = \langle\varphi_1|\varphi\rangle$

FIGURE 4.6 **Projection of φ onto an orthonormal set of eigenfunctions in Hilbert space.**

·4 to the one-dimensional box Problem (4.15). This means that any function φ in this Hilbert space may be expanded in a series of the sequence $\{\varphi_n\}$.

$$\varphi(x) = \sum_{n=1}^{\infty} a_n \varphi_n(x) \tag{4.33}$$

·1 The geometrical interpretation of this relation is depicted in Fig. 4.6. The coefficient a_n is the projection of φ onto the vector φ_n. To see this, first we state a fact to be illustrated in the next section. The *basis* vectors $\{\varphi_n\}$ comprise an orthogonal set. That is,

$$\langle\varphi_n|\varphi_{n'}\rangle = 0 \qquad (n \neq n') \tag{4.34}$$

2 Furthermore, φ_n is a unit vector; that is, it has unit "length"

$$\langle\varphi_n|\varphi_n\rangle = \|\varphi_n\|^2 = 1 \tag{4.35}$$

2: These latter two statements may be combined into the single equation

$$\langle\varphi_n|\varphi_{n'}\rangle = \delta_{n,n'} \tag{4.36}$$

The symbol $\delta_{n,n'}$ is called the *Kronecker delta* and is defined by

$$\delta_{n,n'} = 0 \quad \text{for } n \neq n', \qquad \delta_{n,n'} = 1 \quad \text{for } n = n' \tag{4.37}$$

Any sequence of functions that obeys (4.36) is called an *orthonormal set.*

To show that a_n is the projection of φ into φ_n, we first rewrite (4.33) in Dirac notation.

$$|\varphi\rangle = \sum_n |a_n \varphi_n\rangle \tag{4.38}$$

Then we multiply from the left by $\langle \varphi_{n'}|$ and use the relation (4.36).

$$\langle \varphi_{n'} | \varphi \rangle = \sum_n \langle \varphi_{n'} | a_n \varphi_n \rangle$$

$$= \sum_n a_n \langle \varphi_{n'} | \varphi_n \rangle = \sum_n a_n \delta_{n,n'} = a_{n'} \tag{4.39}$$

$$a_{n'} = \langle \varphi_{n'} | \varphi \rangle$$

The coefficient $a_{n'}$ is the inner product between the basis vector $\varphi_{n'}$ and the vector φ. Since $\varphi_{n'}$ is a "unit" vector, $a_{n'}$ is the projection of φ onto $\varphi_{n'}$ (Fig. 4.6). The student should recognize (4.33) to be a discrete Fourier series representation of φ, in terms of the trigonometric sequence (4.15).

Delta-Function Orthogonality

We will continue with the use of the labels $\mathfrak{H}_1$ and $\mathfrak{H}_2$ to denote the two Hilbert spaces defined by (4.30) and (4.31), respectively. As stated previously, the sequence $\{\varphi_n\}$ given by (4.15) "spans" $\mathfrak{H}_1$. The sequence $\{\varphi_n\}$ is a basis of $\mathfrak{H}_1$. What are the vectors which span $\mathfrak{H}_2$? The answer is: the eigenfunctions of the momentum operator $\hat{p}$,

$$\varphi_k(x) = \frac{1}{\sqrt{2\pi}} e^{ikx} \tag{4.40}$$

Let us see if this (continuous) set of functions is an orthogonal set. Toward these ends we form the inner product

$$\langle \varphi_k | \varphi_{k'} \rangle = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ix(k'-k)}\, dx = \delta(k' - k) \tag{4.41}$$

$\underline{\delta(y) = 0 , \forall y \neq 0}$

It follows that the inner product between any two distinct eigenvectors of the operator $\hat{p}$ vanishes.

Any function in $\mathfrak{H}_2$ may be expanded in terms of the eigenvectors $\{\varphi_k\}$. Since this sequence comprises a continuous set, the expansion is not a discrete sum as in (4.33), but an integral. If $\varphi(x)$ is any element of $\mathfrak{H}_2$, then since $\{\varphi_k\}$ spans this space, one may write

$$\varphi(x) = \int_{-\infty}^{\infty} b(k) \varphi_k(x)\, dk \tag{4.42}$$

This is the Fourier integral representation of $\varphi(x)$. Again, the coefficients of ex-
1 pansion $b(k)$ is the projection of φ_k onto $\varphi(x)$. To exhibit this fact, we first rewrite the
last integral in the form

$$|\varphi\rangle = \int_{-\infty}^{\infty} dk\,|b(k)\varphi_k\rangle \tag{4.43}$$

Again, if this equation is compared to (4.38), we see how the sum over discrete a_n
values is replaced by an integration over the continuum of $b(k)$ values. If we now multi-
2 ply (4.43) from the left with $\langle\varphi_{k'}|$, there results

$$\begin{aligned} \langle\varphi_{k'}|\varphi\rangle &= \int_{-\infty}^{\infty} dk\langle\varphi_{k'}|b(k)\varphi_k\rangle = \int_{-\infty}^{\infty} dk\,b(k)\langle\varphi_{k'}|\varphi_k\rangle \\ &= \int_{-\infty}^{\infty} dk\,b(k)\delta(k'-k) = b(k') \end{aligned} \tag{4.44}$$

The coefficient of expansion $b(k')$ is the inner product between $\varphi_{k'}$ and φ, hence it
3 may be termed a projection of φ onto $\varphi_{k'}$. But $\varphi_{k'}$ does not appear to be a "unit"
vector. Indeed, the vector φ_k is infinitely long.

$$\|\varphi_k\|^2 = \langle\varphi_k|\varphi_k\rangle = \delta(0) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dx = \infty \tag{4.45}$$

3. Although this disqualifies the set $\{\varphi_k\}$ for membership in $\mathfrak{H}_2$, they nevertheless span the space. They comprise a valid set of basis vectors and the projection of any function in $\mathfrak{H}_2$ onto any member of the basis $\{\varphi_k\}$ gives a finite result. If φ is any function in $\mathfrak{H}_2$, then

$$\langle\varphi_k|\varphi\rangle < \infty \tag{4.46}$$

The functions $\{\varphi_k\}$ may, through proper renormalization, be cast in a form which allows them to be members of $\mathfrak{H}_2$. (See Problem 4.6.)

PROBLEMS

4.6 Consider the functions

$$\varphi_k = \frac{1}{\sqrt{L}}\, e^{ikx}$$

defined over the interval $(-L/2, +L/2)$.

(a) Show that these functions are all normalized to unity and maintain this normalization in the limit $L \to \infty$.

(b) Show that these functions comprise an orthogonal set in the limit $L \to \infty$.

4.7 State to which space each of the functions listed belongs, $\mathfrak{H}_1$ or $\mathfrak{H}_2$.

(a) $f_1 = (x^5 - x^4 - Lx^4 + Lx^3)/(x - 2L)$

(b) $f_2 = (\sin x)e^{-x^2}$

(c) $f_3 = \sqrt{\ln[x(x - L) + 1]}$

(d) $f_4 = \sin 2n\pi[x(x - L) + 1], \quad n = 0, 1, 2, \ldots$

(e) $f_5 = e^{i\alpha x}(x^2 + a^2)^{-1}$

(f) $f_6 = x^{10}e^{-x^2}$

(g) $f_7 = 1/\sin kx$

4.8 The function

$$g(x) = x(x - L)e^{ikx}$$

is in $\mathfrak{H}_1$. Calculate the coefficients of expansion, a_n, of this function, in the series representation (4.33), in terms of the constants L and k. Use the basis functions (4.15).

4.9 Two vectors ψ and φ in a Hilbert space are orthogonal. Show that their lengths obey the Pythagorean theorem,

$$\|\psi + \varphi\|^2 = \|\psi\|^2 + \|\varphi\|^2$$

4.10 Consider a free particle moving in one dimension. The state functions for this particle are all elements of $\mathfrak{H}_2$. Show that the expectation of the momentum $\langle p_x \rangle$ vanishes in any state that is purely real ($\psi^* = \psi$). Does this property hold for $\langle H \rangle$? Does it hold for $\langle x \rangle$?

4.5 HERMITIAN OPERATORS

The average of an observable A for a system in the state $\psi(x, t)$ is given by (3.32). In Dirac notation this equation appears as (in one dimension)

$$\langle A \rangle = \int \psi^*(x, t)\hat{A}\psi(x, t)\,dx = \langle \psi \,|\, \hat{A}\psi \rangle \tag{4.47}$$

Since t is a fixed parameter in this equation, we may conclude that the formula gives the expectation of A at the time t. Now one may ask: What are the possible state functions for a particle moving in one dimension at a given instant of time? The answer is: any function in $\mathfrak{H}_2$. For example, the particle could be in any of the following states at some specified time:

$$\psi_1 = Be^{-x/a^2}, \qquad \psi_2 = \frac{Ce^{ikx}}{x}, \qquad \psi_3 = \frac{iD}{\sqrt{x^2 + a^2}} \tag{4.48}$$

where B, C, and D are normalization constants. Again consider the observable A. If the average of this observable is calculated in any of these states (that is, any

1. $\hat{A}\psi$ is not related in any way to the eigenvalue equation, unless we know explicitly that ψ is an eigenfunction of $\hat{A}$. Since $\psi \in \mathfrak{H}$ and $\hat{A}$ is defined over $\mathfrak{H}$ one can regard $\hat{A}$ as a transformation operator in $\mathfrak{H}$ which transforms the element $\psi \in \mathfrak{H}$ into another element $(\hat{A}\psi) \in \mathfrak{H}$. Therefore $\langle \psi_l | \hat{A} \psi_n \rangle$ is not in any way related to $\langle \hat{A} \rangle$, it is just a projection of $|\hat{A}\psi_n\rangle$ onto $\langle \psi_l |$ which is equivalent to $\langle \psi_l | \hat{A} \psi_n \rangle \equiv \int \psi_l^* \hat{A} \psi_n \, dx$.

2. Always keep the mental relation between $\hat{A} \in \mathfrak{H} \sim a \in \mathbb{C}$ and $\hat{A}^\dagger \in \mathfrak{H} \sim a^* \in \mathbb{C}$ when $\hat{A} \equiv \hat{A}^\dagger \equiv$ Hermitian Operator.

In physics we live in the real $\mathfrak{H}$ which is related to the real axis of $\mathbb{C}$. $\boxed{!?}$?

2. member of $\mathfrak{H}_2$), the result must be a real number. This is a property that we demand an operator have if it is to qualify as the operator corresponding to a physical observable. The object $\langle\psi|\hat{A}\psi\rangle$ must be real for all ψ in $\mathfrak{H}_2$. When working with the one-dimensional box problem, $\langle\psi|\hat{A}\psi\rangle$ must be real for all ψ in $\mathfrak{H}_1$. For example, if $\hat{H}$ is the operator corresponding to energy, then

$$\langle E\rangle = \langle\psi|\hat{H}\psi\rangle = -\int_0^L \frac{\psi^*\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi\,dx \tag{4.49}$$

must be real for any state function ψ in $\mathfrak{H}_1$.

3 These observations give rise to the following rule: In quantum mechanics one requires that the eigenvalues of an operator corresponding to a physical observable be real numbers. In this section we discuss the class of operators that have this property. They are called *Hermitian operators* and are a cornerstone in the theory of quantum mechanics.

1. **The Hermitian Adjoint**

To understand what a Hermitian operator is, we must first understand what the *Hermitian adjoint* of an operator is. Consider the operator $\hat{A}$. The Hermitian adjoint of $\hat{A}$ is written $\hat{A}^\dagger$. Under most circumstances, it is an entirely different operator from $\hat{A}$. For instance, the Hermitian adjoint of the complex number c is the complex conjugate of c. That is,

$$c^\dagger = c^* \tag{4.50}$$

1 How is the Hermitian adjoint defined? First, let us agree that an operator is defined over a specific Hilbert space, $\mathfrak{H}$. Also if $\hat{A}$ is the operator and ψ is any element of $\mathfrak{H}$, then $\hat{A}\psi$ is also in $\mathfrak{H}$. For any two elements of this space, say ψ_l and ψ_n, we can form the inner product

$$\langle\psi_l|\hat{A}\psi_n\rangle \tag{4.51}$$

2 Suppose there is another operator, $\hat{A}^\dagger$, also defined over $\mathfrak{H}$, for which

$$\langle\hat{A}^\dagger\psi_l|\psi_n\rangle = \langle\psi_l|\hat{A}\psi_n\rangle \tag{4.52}$$

† 3 Suppose further that this equality holds for *all* ψ_l and ψ_n in $\mathfrak{H}$. Then $\hat{A}^\dagger$ is called the *Hermitian adjoint* of $\hat{A}$. To find the Hermitian adjoint of an operator $\hat{A}$, we have to find the object $\hat{A}^\dagger$ that fits (4.52) for all ψ_l and ψ_n. Consider $\hat{A} = a$, a complex number. Then

$$\langle a^\dagger\psi_l|\psi_n\rangle = \langle\psi_l|a\psi_n\rangle = a\langle\psi_l|\psi_n\rangle = \langle a^*\psi_l|\psi_n\rangle \tag{4.53}$$

Equating the first and the last terms, we see that $a^\dagger = a^*$. As a second example, consider the operator

$$\hat{D} = \frac{\partial}{\partial x} \tag{4.54}$$

defined in $\mathfrak{H}_2$. Then

$$\begin{aligned} \langle\psi_l|\hat{D}\psi_n\rangle &= \int_{-\infty}^{\infty} dx\,\psi_l{}^* \frac{\partial}{\partial x}\psi_n = [\psi_l{}^*\psi_n]_{-\infty}^{+\infty} - \int_{-\infty}^{\infty} dx\left(\frac{\partial}{\partial x}\psi_l{}^*\right)\psi_n \\ &= \langle -\hat{D}\psi_l|\psi_n\rangle \end{aligned} \tag{4.55}$$

The "surface" term is zero since ψ_l and ψ_n are elements of $\mathfrak{H}_2$. Thus we find

$$\hat{D}^\dagger = -\hat{D} \tag{4.56}$$

For some cases we will find that the Hermitian adjoint of an operator is the operator itself. For such an operator $\hat{A}$, we may write

$$\hat{A}^\dagger = \hat{A} \tag{4.57}$$

In terms of the defining equation (4.52), this implies that for all ψ_l and ψ_n in $\mathfrak{H}$ (over which $\hat{A}$ is defined),

$$\langle\psi_l|\hat{A}\psi_n\rangle = \langle\hat{A}\psi_l|\psi_n\rangle \tag{4.58}$$

Operators that have this property are called *Hermitian operators*. The simplest example of a Hermitian operator is any real number a, since

$$\langle\psi_l|a\psi_n\rangle = \langle a\psi_l|\psi_n\rangle \tag{4.59}$$

If $\hat{A}$ and $\hat{B}$ are two Hermitian operators, is the product operator $\hat{A}\hat{B}$ Hermitian? This is most simply answered with the aid of Problem 4.11(b), according to which

$$(\hat{A}\hat{B})^\dagger = \hat{B}^\dagger\hat{A}^\dagger \tag{4.60}$$

If $\hat{A}$ and $\hat{B}$ are Hermitian, then

$$(\hat{A}\hat{B})^\dagger = \hat{B}\hat{A} \tag{4.61}$$

and $\hat{A}\hat{B}$ is not (necessarily) Hermitian. What about $\hat{A}\hat{B} + \hat{B}\hat{A}$?

$$\begin{aligned} (\hat{A}\hat{B} + \hat{B}\hat{A})^\dagger &= \hat{B}^\dagger\hat{A}^\dagger + \hat{A}^\dagger\hat{B}^\dagger = \hat{B}\hat{A} + \hat{A}\hat{B} \\ &= \hat{A}\hat{B} + \hat{B}\hat{A} \end{aligned} \tag{4.62}$$

It follows that if $\hat{A}$ and $\hat{B}$ are both Hermitian, so is the bilinear form $(\hat{A}\hat{B} + \hat{B}\hat{A})$.

Is the square of a Hermitian operator Hermitian?

$$(\hat{A}^2)^\dagger = (\hat{A}\hat{A})^\dagger = \hat{A}^\dagger\hat{A}^\dagger = \hat{A}\hat{A} = (\hat{A})^2 \tag{4.63}$$

1 If $\hat{A}$ and $\hat{B}$ are Hermitian, $\hat{A}\hat{B}$ is not necessarily Hermitian and $(\hat{A}\hat{B})^{\dagger} = \hat{B}^{\dagger}\hat{A}^{\dagger} = \hat{B}\hat{A}$ and in this case $(\hat{A}\hat{B}) \not\equiv (\hat{A}\hat{B})^{\dagger} \equiv \hat{B}\hat{A}$

$\Rightarrow \hat{A}\hat{B} - \hat{B}\hat{A} = \hat{C} \neq 0$.

2 Suppose $\hat{A}\hat{B} - \hat{B}\hat{A} = 0$, $\hat{A}\hat{B} = \hat{B}\hat{A} = (\hat{A}\hat{B})^{\dagger}$ i.e $(\hat{A}\hat{B})$ is Hermitian.

$[\hat{A}, \hat{B}] = 0$, and $\hat{A}, \hat{B}$ commute

and the physical observables A and B can be measured or observed simultaneously i.e A and B can send information at the same time.

(Take my breath away) Berlin

watching every motion

(Sat. 5-9-1992 21.35 GMT)

Unforgetable

Irruption

one way take it to the future

The answer is yes. Another way of doing this problem is as follows. Look at the inner product,

$$\langle \psi_l | \hat{A}\hat{A}\psi_n \rangle = \langle \hat{A}\psi_l | \hat{A}\psi_n \rangle = \langle \hat{A}\hat{A}\psi_l | \psi_n \rangle \tag{4.64}$$

The first equality follows because $\hat{A}\psi_n$ is in $\mathfrak{H}$ and $\hat{A}$ is Hermitian, while the second equality follows simply because $\hat{A}$ is Hermitian. Comparing the first and third terms shows that $\hat{A}^2$ is Hermitian.

The Momentum and Energy Operators

Let us test the momentum operator $\hat{p}$ and see if it is Hermitian. For the free-particle case, $\hat{p}$ is Hermitian if for all ψ_l and ψ_n in $\mathfrak{H}_2$,

$$\langle \psi_l | \hat{p}\psi_n \rangle = \langle \hat{p}\psi_l | \psi_n \rangle \tag{4.65}$$

Developing the left-hand side, we have

$$\begin{aligned} \int_{-\infty}^{\infty} \psi_l^* \left(-i\hbar \frac{\partial}{\partial x} \psi_n \right) dx &= -i\hbar [\psi_l^* \psi_n]_{-\infty}^{\infty} + i\hbar \int_{-\infty}^{\infty} \left(\frac{\partial}{\partial x} \psi_l^* \right) \psi_n \, dx \\ &= \int_{-\infty}^{\infty} \left(-i\hbar \frac{\partial}{\partial x} \psi_l \right)^* \psi_n \, dx = \langle \hat{p}\psi_l | \psi_n \rangle \end{aligned} \tag{4.66}$$

This technique is, by and large, the principal method by which a specific operator is shown to be Hermitian.

Having shown that $\hat{p}$ is Hermitian, it follows that the free-particle Hamiltonian, $\hat{H}$, is Hermitian.

$$\hat{H} = \frac{\hat{p}^2}{2m} \tag{4.67}$$

$$\hat{H}^\dagger = \left(\frac{\hat{p}^2}{2m} \right)^\dagger = \frac{\hat{p}^2}{2m} = \hat{H} \tag{4.68}$$

[Recall (4.63).] For a particle in a potential field $V(x)$,

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(x) \tag{4.69}$$

Since $V(x)$ is a real function that merely multiplies (say in $\mathfrak{H}_2$), it is Hermitian.

$$\begin{aligned} \langle \psi_l | V\psi_n \rangle &= \int_{-\infty}^{\infty} \psi_l^* V \psi_n \, dx = \int_{-\infty}^{\infty} V \psi_l^* \psi_n \, dx \\ &= \int (V\psi_l)^* \psi_n \, dx = \langle V\psi_l | \psi_n \rangle \end{aligned} \tag{4.70}$$

It follows that $\hat{H}$ as given by (4.69) is Hermitian.

PROBLEMS

4.11 (a) Show that $(aA + bB)^\dagger = a^*A^\dagger + b^*B^\dagger$.

(b) Show that $(\hat{A}\hat{B})^\dagger = \hat{B}^\dagger\hat{A}^\dagger$.

(c) What is the Hermitian adjoint of the real number a?

(d) What is the Hermitian adjoint of $\hat{D}^2$? [See (4.54).]

(e) What is the Hermitian adjoint of $(\hat{A}\hat{B} - \hat{B}\hat{A})$?

(f) What is the Hermitian adjoint of $(\hat{A}\hat{B} + \hat{B}\hat{A})$?

(g) What is the Hermitian adjoint of $i(\hat{A}\hat{B} - \hat{B}\hat{A})$?

(h) What is $(A^\dagger)^\dagger$?

(i) What is $(\hat{A}^\dagger\hat{A})^\dagger$?

4.12 If $\hat{A}$ and $\hat{B}$ are both Hermitian, which of the following three operators are Hermitian?

(a) $i(\hat{A}\hat{B} - \hat{B}\hat{A})$.

(b) $(\hat{A}\hat{B} - \hat{B}\hat{A})$.

(c) $\left(\dfrac{\hat{A}\hat{B} + \hat{B}\hat{A}}{2}\right)$.

(d) If $\hat{A}$ is not Hermitian, is the product $\hat{A}^\dagger A$ Hermitian?

(e) If $\hat{A}$ corresponds to the observable A, and $\hat{B}$ corresponds to B, what is a "good" (i.e., Hermitian) operator that corresponds to the physically observable product AB?

4.13 If $\hat{A}$ is Hermitian, show that

$$\langle \hat{A}^2 \rangle \geq 0$$

Answer (in $\mathfrak{H}_2$)

$$\langle \hat{A}^2 \rangle = \int_{-\infty}^{\infty} \psi^* \hat{A}^2 \psi \, dx = \int_{-\infty}^{\infty} (\hat{A}\psi)^* \hat{A}\psi \, dx$$

$$= \int_{-\infty}^{\infty} |\hat{A}\psi|^2 \, dx \geq 0$$

4.14 If $\hat{A}$ is Hermitian, show that $\langle A \rangle$ is real; that is, show that $\langle A \rangle^* = \langle A \rangle$.

4.15 For a particle moving in one dimension, show that the operator $\hat{x}\hat{p}$ is not Hermitian. Construct an operator which corresponds to this physically observable product that is Hermitian.

4.6 PROPERTIES OF HERMITIAN OPERATORS

The first property of Hermitian operators we wish to establish is that their eigenvalues are real. Let $\hat{A}$ be a Hermitian operator. Let $\{\varphi_n\}$ and $\{a_n\}$ represent, respectively, the eigenfunctions and eigenvalues of the operator $\hat{A}$.

(4.71) $$\hat{A}\varphi_n = a_n\varphi_n$$

In Dirac notation

(4.72) $$|\hat{A}\varphi_n\rangle = |a_n\varphi_n\rangle \quad \text{or equivalently} \quad \hat{A}|\varphi_n\rangle = a_n|\varphi_n\rangle$$

(4.11) (a) $\langle (a\hat{A}+b\hat{B})^{\dagger}\psi_l|\psi_n\rangle = \langle\psi_l|(a\hat{A}+b\hat{B})\psi_n\rangle =$

$\langle\psi_l|a\hat{A}\psi_n\rangle + \langle\psi_l|b\hat{B}\psi_n\rangle = a\langle\psi_l|\hat{A}\psi_n\rangle + b\langle\psi_l|\hat{B}\psi_n\rangle =$

$a\langle\hat{A}^{\dagger}\psi_l|\psi_n\rangle + b\langle\hat{B}^{\dagger}\psi_l|\psi_n\rangle = \langle a^{*}\hat{A}^{\dagger}\psi_l|\psi_n\rangle + \langle b^{*}\hat{B}^{\dagger}\psi_l|\psi_n\rangle =$

$\langle(a^{*}\hat{A}^{\dagger}+b^{*}\hat{B}^{\dagger})\psi_l|\psi_n\rangle = \langle\psi_l|(a\hat{A}+b\hat{B})\psi_n\rangle$ ■

(b) $\langle(\hat{A}\hat{B})^{\dagger}\psi_l|\psi_n\rangle = \langle\psi_l|\hat{A}\hat{B}|\psi_n\rangle$, let $\hat{B}|\psi_n\rangle = |\psi_n'\rangle \Rightarrow$

$\langle\psi_l|\hat{A}\psi_n'\rangle = \langle\hat{A}^{\dagger}\psi_l|\hat{B}\psi_n\rangle$, let $\langle\hat{A}^{\dagger}\psi_l| = \langle\psi_l'| \Rightarrow$

$\langle\psi_l'|\hat{B}\psi_n\rangle = \langle\hat{B}^{\dagger}\psi_l'|\psi_n\rangle = \langle\hat{B}^{\dagger}\hat{A}^{\dagger}\psi_l|\psi_n\rangle$ i.e $(\hat{A}\hat{B})^{\dagger} = \hat{B}^{\dagger}\hat{A}^{\dagger}$

(c) $a^{\dagger} = a^{*} = a \in \mathbb{R}$

(d) $\langle(\hat{D}^2)^{\dagger}\psi_l|\psi_n\rangle = \langle\psi_l|\hat{D}|\hat{D}\psi_n\rangle = \langle\psi_l|\hat{D}|\psi_n'\rangle = \langle\hat{D}^{\dagger}\psi_l|\psi_n'\rangle =$

$-\langle D\psi_l|\psi_n'\rangle = -\langle\psi_l'|\hat{D}\psi_n\rangle = -\langle\hat{D}^{\dagger}\psi_l'|\psi_n\rangle = -1\times-1\,\langle D\psi_l'|\psi_n\rangle =$

$\langle\hat{D}^2\psi_l|\psi_n\rangle = \langle(\hat{D}^2)^{\dagger}\psi_l|\psi_n\rangle \Rightarrow (\hat{D}^2)^{\dagger} = \hat{D}^2$.

* another way from (b) $(\hat{D}^2)^{\dagger} = (\hat{D}\hat{D})^{\dagger} = (\hat{A}\hat{B})^{\dagger} = \hat{B}^{\dagger}\hat{A}^{\dagger} = (-D)(-D) = D^2$.

(e) $\langle((\hat{A}\hat{B})-\hat{B}\hat{A})^{\dagger}\psi_l|\psi_n\rangle = \langle\psi_l|(AB-BA)\psi_n\rangle = \langle\psi_l|AB\psi_n\rangle - \langle\psi_l|BA\psi_n\rangle =$

$\langle\hat{B}^{\dagger}\hat{A}^{\dagger}\psi_l|\psi_n\rangle - \langle\hat{A}^{\dagger}\hat{B}^{\dagger}\psi_l|\psi_n\rangle = \langle(\hat{B}^{\dagger}\hat{A}^{\dagger}-\hat{A}^{\dagger}\hat{B}^{\dagger})\psi_l|\psi_n\rangle \Rightarrow$

$(\hat{A}\hat{B}-\hat{B}\hat{A})^{\dagger} = \hat{B}^{\dagger}\hat{A}^{\dagger} - \hat{A}^{\dagger}\hat{B}^{\dagger} = (AB)^{\dagger} - (BA)^{\dagger}$ ■

(f) $(AB+BA)^{\dagger} = (AB)^{\dagger} + (BA)^{\dagger} = \hat{B}^{\dagger}\hat{A}^{\dagger} + \hat{A}^{\dagger}\hat{B}^{\dagger}$ □

The operator $\dagger$ is linear w.r to addition.

(g) $i(AB-BA) = i[A,B] = iC \Rightarrow \langle(iC)^{\dagger}\psi_l|\psi_n\rangle = \langle\psi_l|iC\psi_n\rangle$

$= i\langle\psi_l|C\psi_n\rangle = i\langle\hat{C}^{\dagger}\psi_l|\psi_n\rangle = \langle -i\hat{C}^{\dagger}\psi_l|\psi_n\rangle \Rightarrow (iC)^{\dagger} = -iC^{\dagger}$

$[i(AB-BA)]^{\dagger} = i(BA-AB) = -i[A,B]^{\dagger}$ ■

(h) $(A^{\dagger})^{\dagger} = (B)^{\dagger}$. $\langle A^{\dagger}\psi_l|\psi_n\rangle = \langle\psi_l|A\psi_n\rangle = \langle B\psi_l|\psi_n\rangle =$

$\langle\psi_l|\hat{B}^{\dagger}\psi_n\rangle = \langle\psi_l|A\psi_n\rangle \Rightarrow (\hat{A}^{\dagger})^{\dagger} = (\hat{B})^{\dagger} = \hat{A}$

(i) $(\hat{A}^{\dagger}\hat{A})^{\dagger} = (\hat{B}\hat{C})^{\dagger} = \hat{C}^{\dagger}\hat{B}^{\dagger} = \hat{A}^{\dagger}(\hat{A}^{\dagger})^{\dagger} = \hat{A}^{\dagger}\hat{A} \Rightarrow$

$[(\hat{A}^{\dagger}\hat{A})^{\dagger} = \hat{A}^{\dagger}\hat{A}]$ which is a physical Hermitian operator.

for any operator $\hat{A}$ defined over Hilbert Space. ■

(4.12) (a) from (9) $(i(AB-BA))^{\dagger} = -i(AB-BA)^{\dagger} = -i((AB)^{\dagger} - (BA)^{\dagger}) =$

$-i(\hat{B}^{\dagger}\hat{A}^{\dagger} - \hat{A}^{\dagger}\hat{B}^{\dagger}) = -i(\hat{B}\hat{A} - \hat{A}\hat{B}) = i(\hat{A}\hat{B} - \hat{B}\hat{A}) \Rightarrow$

$(iC)^{\dagger} = iC = i(\hat{A}\hat{B} - \hat{B}\hat{A})$.

Therefore, $\hat{A}$, $\hat{B}$ & $i[A,B]$ are Hermitian operators.

(b) $(AB-BA)^{\dagger} = (AB)^{\dagger} - (BA)^{\dagger} = -((BA)^{\dagger} - (AB)^{\dagger}) = -(AB-B$

$\Rightarrow$ not Hermitian.

(c) $\left(\frac{\hat{A}\hat{B}+\hat{B}\hat{A}}{2}\right)^{\dagger} = \frac{1}{2}(\hat{A}\hat{B}+\hat{B}\hat{A})^{\dagger} = \frac{1}{2}((AB)^{\dagger} + (BA)^{\dagger}) =$

$\frac{1}{2}((BA)^{\dagger} + (AB)^{\dagger}) = \frac{1}{2}(\hat{A}\hat{B} + \hat{B}\hat{A}) \Rightarrow$ Hermitian.

$\left(\frac{1}{2}[A,B]_{+}\right)^{\dagger} = \frac{1}{2}[A,B]_{+}$

(d) from (i) $(\hat{A}^{\dagger}\hat{A})^{\dagger} = \hat{A}^{\dagger}\hat{A}$ is Hermitian operator even though the operator $\hat{A}$ is not Hermitian.

(e) $(\hat{A})^{\dagger} = \hat{A}$, $(\hat{B})^{\dagger} = \hat{B} \Rightarrow (\hat{A}\hat{B})^{\dagger} = \hat{B}^{\dagger}\hat{A}^{\dagger} = \hat{B}\hat{A} = \hat{A}\hat{B}$

$(\hat{A}\hat{B})^{\dagger} = (\hat{A}\hat{B})$ because $(\hat{A}\hat{B})$ is for a physically observable.

$\hat{A} = a\hat{B}$, at most $a \in \mathbb{R}$

(4.13) $\langle \hat{A}^2 \rangle = \langle \psi | A A | \psi \rangle = \langle A\psi | A\psi \rangle = \int_{-\infty}^{\infty} A\psi^* A\psi \, dx$

$\hat{A}$ is Hermitian $\Rightarrow \hat{A} \neq 0$, $\psi \in \mathbb{C}$ in general $\Rightarrow$

$|\hat{A}\psi|^2 \geq 0$, $\hat{A}\psi = a\psi = 0 \Leftrightarrow a = 0$ because $\hat{A}\psi = a\psi$

$\int A\psi^* A\psi \, dx = \int a\psi^* a\psi \, dx = a^2 \int_{-\infty}^{\infty} \psi^* \psi \, dx = a^2 \times 1 = a^2 \geq 0$

(4.14) $\langle A \rangle = \langle \psi | \hat{A}\psi \rangle$ but from Dirac Notation

$(\langle \varphi | \psi \rangle)^* = \langle \psi | \varphi \rangle \rightarrow$.

$\langle A \rangle^* = (\langle \psi | \hat{A}\psi \rangle)^* = \langle \hat{A}\psi | \psi \rangle = \langle \psi | A\psi \rangle$

this is because $\hat{A}$ is Hermitian.

$\rightarrow (\langle A \rangle)^* = \langle A \rangle$

1 Multiplying from the left with $\langle\varphi_n|$ gives

$$\langle\varphi_n|\hat{A}\varphi_n\rangle = \langle\varphi_n|a_n\varphi_n\rangle = a_n\langle\varphi_n|\varphi_n\rangle \tag{4.73}$$

2 Since $\hat{A}$ is Hermitian, we can write the left-hand side as

$$\langle\hat{A}\varphi_n|\varphi_n\rangle = \langle a_n\varphi_n|\varphi_n\rangle = a_n{}^*\langle\varphi_n|\varphi_n\rangle \tag{4.74}$$

3 Equating the last terms in the latter two equations gives

$$a_n{}^* = a_n \tag{4.75}$$

and a_n is real.

2 The second property of Hermitian operators we wish to establish is that *their*
1 *eigenfunctions are orthogonal.* Again consider (4.72). Now multiply from the left with
another eigenvector of $\hat{A}$, $\langle\varphi_l|$. There results

$$\langle\varphi_l|\hat{A}\varphi_n\rangle = a_n\langle\varphi_l|\varphi_n\rangle \tag{4.76}$$

Since $\hat{A}$ is Hermitian, the left-hand side of this equation can be rewritten

$$\langle\hat{A}\varphi_l|\varphi_n\rangle = a_l{}^*\langle\varphi_l|\varphi_n\rangle = a_l\langle\varphi_l|\varphi_n\rangle \tag{4.77}$$

2 The eigenvalue a_l is real because it is an eigenvalue of a Hermitian operator (i.e., $\hat{A}$). Subtracting the two equations above gives

$$(a_l - a_n)\langle\varphi_l|\varphi_n\rangle = 0 \tag{4.78}$$

3 If $a_l \neq a_n$, this equation says that

$$\langle\varphi_l|\varphi_n\rangle = 0 \tag{4.79}$$

which is the expression of the orthogonality of the set of functions $\{\varphi_n\}$. If these functions are all normalized, then (4.79) may be generalized to read

$$\langle\varphi_l|\varphi_n\rangle = \delta_{ln} \tag{4.80}$$

Thus, the eigenvalues of a Hermitian operator are real, and its eigenfunctions are orthogonal.

PROBLEMS

4.16 Show that if an operator $\hat{B}$ has an eigenvalue $b_1 \neq b_1{}^*$, then $\hat{B}$ is not Hermitian.

4.17 Consider the operator $\hat{C}$,

$$\hat{C}\varphi(x) = \varphi^*(x)$$

(a) Is $\hat{C}$ Hermitian?
(b) What are the eigenfunctions of $\hat{C}$?
(c) What are the eigenvalues of $\hat{C}$?

4.18 Given that the operator $\hat{O}$ annihilates the ket vector $|f\rangle$, that is, $\hat{O}|f\rangle = 0$, what is the value of the bra vector $\langle f|\hat{O}^{\dagger}$? Interpret the meaning of your answer.

4.19 The parallelogram law of geometry states that: the sum of the squares of the diagonals of a parallelogram equals twice the sum of the squares of the sides. Show that this is also true in Hilbert space; that is, if ψ and φ are any two elements of a Hilbert space, then

$$\|\psi + \varphi\|^2 + \|\psi - \varphi\|^2 = 2\|\psi\|^2 + 2\|\varphi\|^2$$

4.20 Show that the standard properties of $\cos\theta$, together with the definition of the inner product between two vectors φ and ψ, in $\mathfrak{H}$, with respective lengths, $\|\varphi\|$ and $\|\psi\|$, imply the Cauchy–Schwartz inequality

$$|\langle\varphi|\psi\rangle| \le \|\varphi\|\,\|\psi\|$$

4.21 Use the Cauchy–Schwartz inequality to prove the triangle inequality

$$\|\varphi + \psi\|^2 \le (\|\varphi\| + \|\psi\|)^2$$

4.22 Construct the squared length of $(\psi - \varphi)$ to show that

$$\|\psi\|^2 + \|\varphi\|^2 \ge 2\,\mathrm{Re}\,\langle\psi|\varphi\rangle$$

4.23 Let the sequence $\{\varphi_n\}$ be an orthonormal basis in $\mathfrak{H}$. Let the sequence $\{\cos\theta_n\}$ represent the angles between the vectors $\{\varphi_n\}$ and an arbitrary element ψ in $\mathfrak{H}$. Using Bessel's inequality,

$$\sum_{n=1}^{\infty} |\langle\varphi_n|\psi\rangle|^2 \le \|\psi\|^2$$

show that

$$\sum_{n=1}^{\infty} \cos^2\theta_n \le 1$$

Under what circumstances does the equality hold?

4.24 Every convergent sequence is also a *Cauchy sequence.* A sequence $\{\varphi_n(x)\}$ is a Cauchy sequence if

$$\lim_{\substack{n\to\infty \\ l\to\infty}} \|\varphi_n - \varphi_l\| = 0$$

A function space $\mathfrak{H}$ is a *complete space* if every Cauchy sequence in $\mathfrak{H}$ converges to an element of $\mathfrak{H}$. This is a requirement that a function space must satisfy in order that it be termed a Hilbert space. (See property 4 after Eq. 4.27.) Show that the space of functions on the unit interval with the property $\varphi(0) = \varphi(1) = 0$ is not a Hilbert space.

4.25 In addition to a complete space, one also defines a *complete sequence.* An orthonormal sequence $\{\varphi_n\}$ is complete in $\mathfrak{H}$ if there is no vector ψ, in $\mathfrak{H}$ of nonzero length ($\|\psi\| > 0$), which is perpendicular to all the elements in the sequence $\{\varphi_n\}$. Show that if $\{\varphi_n\}$ is an orthonormal basis of $\mathfrak{H}$, it is complete in $\mathfrak{H}$.

Answer

Let $\{\varphi_n\}$ be an orthonormal basis of $\mathfrak{H}$. Let ψ be an element of $\mathfrak{H}$ with nonzero length, which is normal to all the elements of $\{\varphi_n\}$. If $\{\varphi_n\}$ is a basis, then we may expand ψ,

$$\psi = \sum a_n \varphi_n = \sum \langle \varphi_n | \psi \rangle \varphi_n$$

But ψ is normal to all φ_n. Therefore, $\langle \varphi_n | \psi \rangle = 0$, which gives $\psi = 0$, so the hypothesis leads to a contradiction, hence the hypothesis is an incorrect statement and there is no such ψ in $\mathfrak{H}$.

* **4.26** Show that any operator $\hat{A}$ may be expressed as the linear combination of a Hermitian and an anti-Hermitian ($\hat{B}^\dagger = -\hat{B}$) operator.

Answer

$$\hat{A} = \left(\frac{\hat{A} + \hat{A}^\dagger}{2}\right) + i\left(\frac{\hat{A} - \hat{A}^\dagger}{2i}\right)$$

[*Note:* $\hat{A} + \hat{A}^\dagger$ and $i(\hat{A} - \hat{A}^\dagger)$ are both Hermitian.]

4.27 Show that the wavefunctions for a particle in a one-dimensional box with walls at $x = 0$ and L satisfy the equality

$$\int_0^L \psi^* \psi_{xx} \, dx = -\int_0^L |\psi_x|^2 \, dx$$

The subscript x denotes differentiation.

4.28 Use the equality proved in Problem 4.27 to establish the following *variational principle*. If the expectation $\int \psi^* \hat{H} \psi \, dx$ is minimum, the normalized wavefunction ψ is the ground state. Specifically, establish the theorem for a particle in a one-dimensional box, assuming real wavefunctions.

Answer

Apart from a constant factor and with the results of Problem 4.27, we may write

$$\langle H \rangle = -\int_0^L \psi^* \psi_{xx} \, dx = \int_0^L {\psi_x}^2 \, dx$$

Let ψ minimize $\langle H \rangle$. Then infinitesimal variation of ψ causes no change in $\langle H \rangle$. Let $\psi \to \psi + \delta\psi$. The variation $\delta\psi$ is an arbitrary infinitesimal function of x that vanishes at $x = 0$ and L. Then

$$\langle H \rangle = \int {\psi_x}^2 \, dx \to \int (\psi_x + \delta\psi_x)^2 \, dx = \langle H \rangle + \delta\langle H \rangle$$

$$\delta\langle H \rangle = 2 \int \psi_x \, \delta\psi_x \, dx = 2 \int \psi_x \frac{d}{dx} \delta\psi \, dx = 0$$

Integrating the last term by parts and dropping the "surface" terms gives

$$\int \psi_{xx} \, \delta\psi \, dx = 0$$

Variation of the normalization statement (both ψ and $\psi + \delta\psi$ are normalized) gives

$$\lambda \int \psi \delta\psi \, dx = 0$$

where λ is an arbitrary undetermined multiplier. Combining the last two equations yields

$$\int_0^L \delta\psi(\psi_{xx} - \lambda\psi) \, dx = 0$$

If this equation is to be satisfied for arbitrary variation of ψ about the minimizing value, we may conclude

$$\psi_{xx} = \lambda\psi$$

It follows that ψ is an eigenstate of $\hat{H}$, in which case $\langle H \rangle$ is an energy eigenvalue which has minimum value for the ground state.

Super nature

- One upon a time

Single Side band

(Narrow Selectivity)

Pilot tone SSB

Syncronous detection

232 fast start

Wave guide

CHAPTER 5

SUPERPOSITION AND COMPATIBLE OBSERVABLES

5.1 *The Superposition Principle*
5.2 *Commutator Relations in Quantum Mechanics*
5.3 *More on the Commutator Theorem*
5.4 *Commutator Relations and the Uncertainty Principle*
5.5 *"Complete" Sets of Commuting Observables*

How Physics is observed?

In this chapter we encounter the superposition principle, which is considered by many to be one of the more fundamental concepts of quantum mechanics. This principle represents one of the basic differences between classical and quantum mechanics and also provides a deeper understanding of the uncertainty principle. Closely related to the superposition principle are the commutator theorem and the notions of compatible observables and simultaneous eigenfunctions.

5.1 THE SUPERPOSITION PRINCIPLE

a strange observation for
a strange superposition.

Ensemble Average

$\psi(x,0) \equiv$ State of the ensemble; and we did not measure at t=0

Consider again a particle in a one-dimensional box. Let us imagine a large number of identical replicas of the system (called an *ensemble* in statistical mechanics), such as described in Section 3.3. If each such box is in the *same* initial state $\psi(x, 0)$, after an interval of time t, each box will again be in a common state $\psi(x, t)$, as shown in Fig. 5.1. Suppose that we ask what the energy of the particle is in each box, at the time t. The laws of nature are such that the energy measured in each of the identical

$\hat{H}\varphi_n = E_n\varphi_n \mapsto \hat{H}\Phi = E\Phi$, $\psi = \sum_n a_n\varphi_n \Rightarrow$ Quantization.

Remember all E's are Generated in G, they are with us

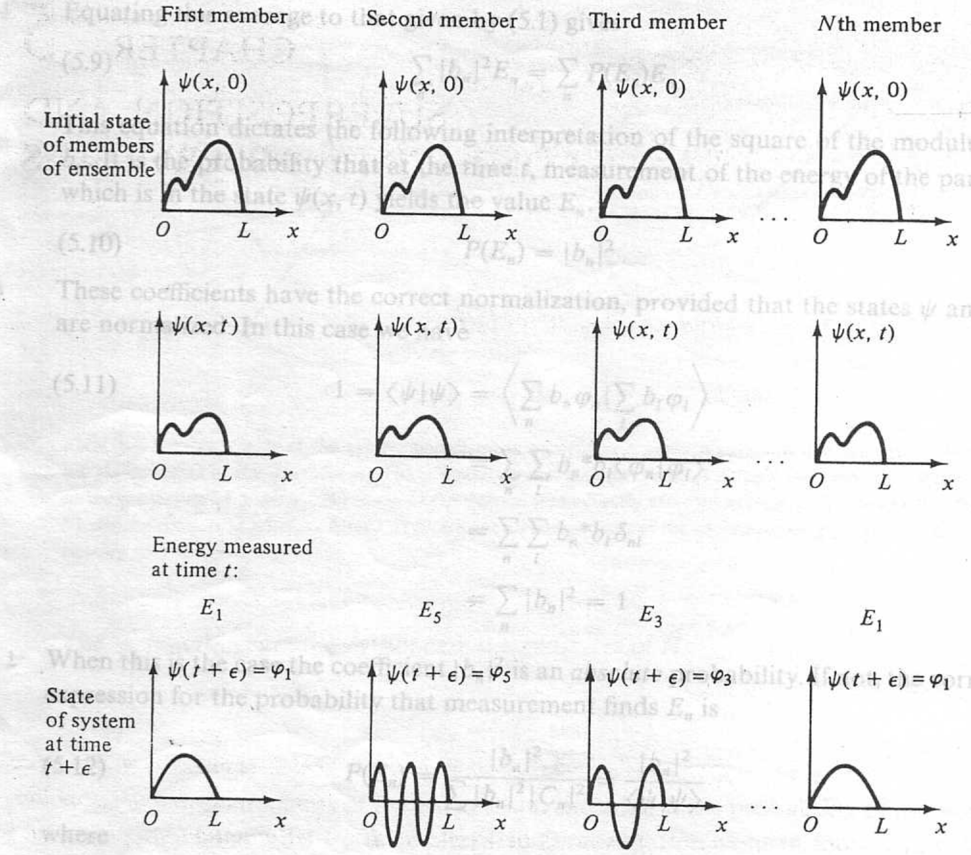

First member
Second member
Third member
Nth member
Initial state of members of ensemble
$\psi(x, 0)$
O
L
x
$\psi(x, t)$
Energy measured at time t:
E_1
E_5
E_3
E_1
State of system at time $t + \epsilon$
$\psi(t + \epsilon) = \varphi_1$
$\psi(t + \epsilon) = \varphi_5$
$\psi(t + \epsilon) = \varphi_3$
$\psi(t + \epsilon) = \varphi_1$

FIGURE 5.1 **Measurement of energy of N identical one-dimensional boxes which comprise an "ensemble." All boxes are in the same state at $t = 0$.**

leaving out

boxes, which are all in the identically same state $\psi(x, t)$, are not the same [save for the case that $\psi(x, 0)$ is an eigenstate of $\hat{H}$].

except

How does one answer the question above: What will the energy be? Since the energy measured at the time t in each box of the ensemble will most likely not be the same, more appropriate questions are: (1) What is the average of the energies measured in all the boxes of the ensemble? (2) If we measure the energy in one box, with what probability will the value, say, E_3 be found? To answer these questions, we first recall that if the probability of finding the value E_n in a given measurement of energy is $P(E_n)$, then the average energy over measurements of all members of the ensemble in the limit as this number becomes large is given by the expression

$$\langle E \rangle = \sum_{\text{all } E_n} P(E_n) E_n \tag{5.1}$$

1 (Recall Eq. 3.34.) This formula holds for all physical observables. For example, the average particle position is given by

$$\langle x\rangle = \int_0^L xP(x)\,dx \tag{5.2}$$

In this case the integral is a sum over the continuum of values x may assume.

2 The quantum mechanical prescription for calculating the average of a dynamical observable in the state ψ is given by the third postulate of quantum mechanics (Section 3.3, Eq. 3.32). Specifically, for the energy we have (in Dirac notation)

$$\langle E\rangle = \langle \psi|\hat{H}\psi\rangle \tag{5.3}$$

3 Let us expand the state ψ in the eigenstates of $\hat{H}$. These eigenstates obey the equation

$$\hat{H}\varphi_n = E_n\varphi_n \tag{5.4}$$

For the box problem they are explicitly (Eq. 4.15)

$$\varphi_n = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right) \tag{5.5}$$

3 The expansion of ψ in these eigenstates appears as

$$\psi(x,t) = \sum_{n=1}^{\infty} b_n(t)\varphi_n(x) \tag{5.6}$$

2 The state ψ is that of the system at the time t, so that it is, in general, a function of x and t. Since φ_n is a function of x only, the coefficients of expansion b_n may, in general, be functions of time. for (5.5)

1 In Dirac notation, (5.6) appears as

$$|\psi\rangle = \sum_{n=1}^{\infty} |b_n\varphi_n\rangle \tag{5.7}$$

2 Substituting this series into (5.3) gives

$$\begin{aligned}\langle E\rangle &= \left\langle \sum_n b_n\varphi_n \,\middle|\, \hat{H}\sum_l b_l\varphi_l\right\rangle \\ &= \sum_n\sum_l b_n{}^* b_l\langle\varphi_n|\hat{H}\varphi_l\rangle \\ &= \sum_n\sum_l b_n{}^* b_l E_l\langle\varphi_n|\varphi_l\rangle \\ &= \sum_n\sum_l b_n{}^* b_l E_l\delta_{nl} \\ &= \sum_{n=1}^{\infty}|b_n|^2E_n\end{aligned} \tag{5.8}$$

3 Equating this average to that given by (5.1) gives

$$\sum_n |b_n|^2 E_n = \sum_n P(E_n) E_n \tag{5.9}$$

This equation dictates the following interpretation of the square of the modulus of b_n. It is the probability that at the time t, measurement of the energy of the particle which is in the state $\psi(x, t)$ yields the value E_n.

$$P(E_n) = |b_n|^2 \tag{5.10}$$

3 These coefficients have the correct normalization, provided that the states ψ and φ_n are normalized. In this case we have

$$\begin{aligned} 1 = \langle\psi|\psi\rangle &= \left\langle \sum_n b_n \varphi_n \middle| \sum_l b_l \varphi_l \right\rangle \\ &= \sum_n \sum_l b_n{}^* b_l \langle\varphi_n|\varphi_l\rangle \\ &= \sum_n \sum_l b_n{}^* b_l \delta_{nl} \\ &= \sum_n |b_n|^2 = 1 \end{aligned} \tag{5.11}$$

1 When this is the case the coefficient $|b_n|^2$ is an *absolute* probability. If not, the correct expression for the probability that measurement finds E_n is

$$P(E_n) = \frac{|b_n|^2}{\sum |b_n|^2 |C_n|^2} = \frac{|b_n|^2}{\langle\psi|\psi\rangle} \tag{5.12}$$

where

$$|C_n|^2 = \langle\varphi_n|\varphi_n\rangle$$

4 Let us return to the expansion (5.7). The coefficients b_n are calculated in the following manner. Multiply this equation from the left with the bra vector $\langle\varphi_{n'}|$. Owing to the orthonormality of the set $\{\varphi_n\}$, one obtains

$$b_n = \langle\varphi_n|\psi\rangle \tag{5.13}$$

in B

The coefficient b_n is the projection of ψ onto the eigenvector φ_n. The physical in-
1 terpretation of b_n is that $|b_n|^2$ is the probability that measuring E finds the value E_n
2 when the system is in the state ψ. This prescription is true for *any* dynamical observable. Consider the symbolic operator $\hat{F}$

$$\hat{F}\varphi_n = f_n \varphi_n \tag{5.14}$$

3 At a given time t, the system is in the state $\psi(x, t)$. What is the probability that measurement of F at this time finds the value f_3? The state ψ is a superposition state. It is

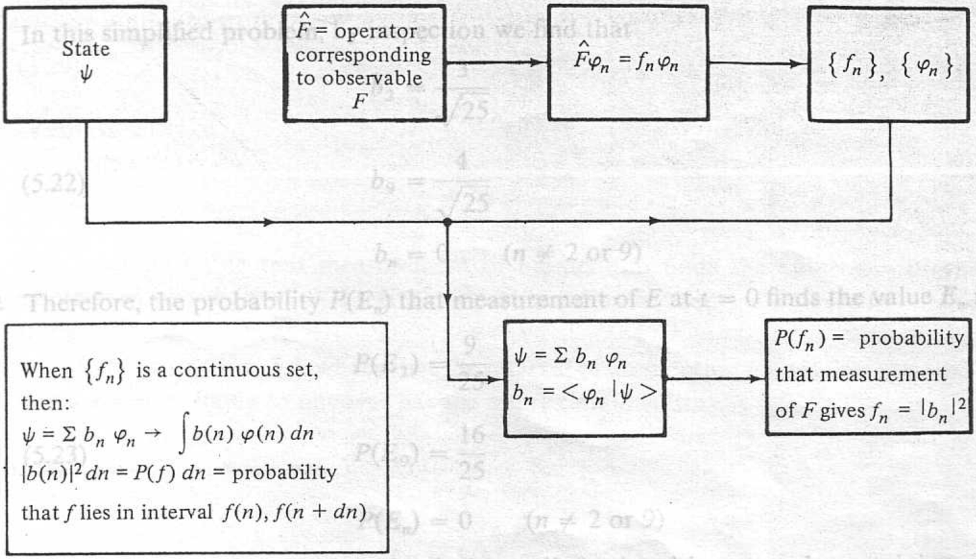

State ψ
$\hat{F}$ = operator corresponding to observable F
$\hat{F}\varphi_n = f_n\varphi_n$
$\{f_n\}, \{\varphi_n\}$
$\psi = \Sigma\, b_n\, \varphi_n$
$b_n = \langle\varphi_n|\psi\rangle$
$P(f_n)$ = probability that measurement of F gives $f_n = |b_n|^2$
When $\{f_n\}$ is a continuous set, then:
$\psi = \Sigma\, b_n\, \varphi_n \rightarrow \int b(n)\, \varphi(n)\, dn$
$|b(n)|^2\, dn = P(f)\, dn$ = probability that f lies in interval $f(n), f(n + dn)$

FIGURE 5.2 Elements of the superposition principle.

composed of the eigenstates of $\hat{F}$. Here we are assuming that the eigenstates of $\hat{F}$ are a basis for the Hilbert space that ψ is in. So we may write

$$\psi = \sum b_n\varphi_n \tag{5.15}$$

$$b_n = \langle\varphi_n|\psi\rangle \tag{5.16}$$

This assumption that an arbitrary state ψ may be represented as a superposition of the eigenstates of a physical observable is the essence of the superposition principle. With $\{\varphi_n\}$ and ψ normalized to unity, the probability that measurement finds the value f_3 is $|b_3|^2$. This procedure is depicted in Fig. 5.2.

Hilbert-Space Interpretation

When we look in Hilbert space, $\{\varphi_n\}$ is one set of vectors and ψ is another vector. The system is in the state ψ. Measurement of F causes the state ψ to fall to one of the φ_n vectors. Chances are that it goes to the φ_n vector to which it is most inclined (in the geometrical sense; see Fig. 5.3).

Consider the following illustrative example. A particle of mass m is in a one-dimensional box of width L. At $t = 0$ the particle is in the state

$$\psi(x, 0) = \frac{3\varphi_2 + 4\varphi_9}{\sqrt{25}} \tag{5.17}$$

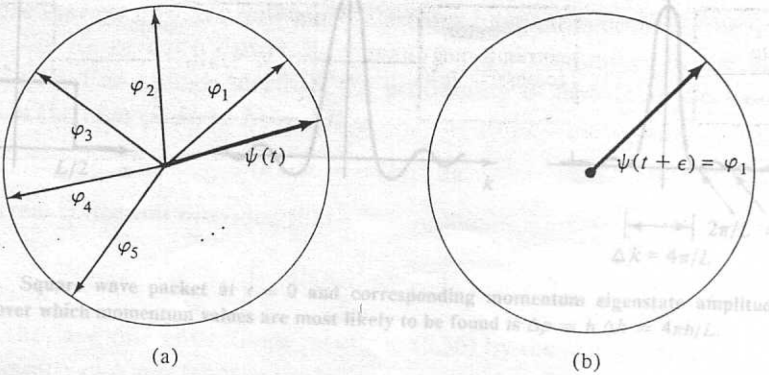


FIGURE 5.3 (a) State of the system before measurement at t, superimposed on the basis $\{\varphi_n\}$, which are the eigenvectors of the operator $\hat{F}$. The probability that measurement of F finds the value f_n is proportional to the projection of ψ on φ_n. (b) State of the system immediately after measurement has found the value f_1. Measurement acts as a "wave filter." It filters out all components of the superposition $\psi(x, t) = \sum b_n(t)\varphi_n(x)$, passing only the φ_1 wave.

The φ_n functions are the orthonormal eigenstates of $\hat{H}$:

$$\varphi_n = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \tag{5.18}$$

What will measurements of E yield at $t = 0$ and what is the probability of finding this value? First let us see if ψ is normalized. In Dirac notation we have, for the state (5.17),

$$|\psi\rangle = \frac{3|\varphi_2\rangle + 4|\varphi_9\rangle}{\sqrt{25}} \tag{5.19}$$

so that

$$\begin{aligned}\langle\psi|\psi\rangle &= \tfrac{1}{25}\{(3\langle\varphi_2| + 4\langle\varphi_9|)(3|\varphi_2\rangle + 4|\varphi_9\rangle)\}\\ &= \tfrac{1}{25}\{9\langle\varphi_2|\varphi_2\rangle + 12\langle\varphi_2|\varphi_9\rangle + 12\langle\varphi_9|\varphi_2\rangle + 16\langle\varphi_9|\varphi_9\rangle\}\\ &= 1\end{aligned} \tag{5.20}$$

and ψ is normalized. The inner products $\langle\varphi_2|\varphi_2\rangle = \langle\varphi_9|\varphi_9\rangle = 1$ while the other two are zero, owing to the orthogonality of the set $\{\varphi_n\}$.

The superposition principle stipulates the following. If we want the probability that measurement finds the value E_n, we must expand ψ in the eigenstates of $\hat{H}$. The square of the magnitude of the coefficient of φ_n is the said probability.

$$\psi = \sum b_n \varphi_n = \frac{3\varphi_2 + 4\varphi_9}{\sqrt{25}} \tag{5.21}$$

In this simplified problem, by inspection we find that

$$b_2 = \frac{3}{\sqrt{25}}$$

(5.22)
$$b_9 = \frac{4}{\sqrt{25}}$$

$$b_n = 0 \qquad (n \neq 2 \text{ or } 9)$$

1 Therefore, the probability $P(E_n)$ that measurement of E at $t = 0$ finds the value E_n is

$$P(E_2) = \frac{9}{25}$$

(5.23)
$$P(E_9) = \frac{16}{25}$$

$$P(E_n) = 0 \qquad (n \neq 2 \text{ or } 9)$$

2 In an ensemble of 2500 identical one-dimensional boxes, each containing an identical particle in the same state $\psi(x, 0)$ given by (5.17), measurement of E at $t = 0$ finds about 900 particles to have energy $E_2 = 4E_1$ and about 1600 particles to have energy $E_9 = 81E_1$.

·2 Is there a chance that in an ensemble of 10^{17} boxes, measurement of E finds
E_2 in all 10^{17} boxes? Yes. This remarkable response carries the philosophical impact
of the superposition principle. Although the state $\psi(x, 0)$ is a precise superposition
of well-defined eigenstates of the observables being measured, one is not *certain* what
1 measurement will yield. There is nothing in classical physics that is similar to this
concept. Any uncertainty in classical physics arises from uncertain initial data. In
2 quantum mechanics, although the initial state $\psi(x, 0)$ is prescribed with perfect
accuracy, one is never certain in which eigenstate, φ_n, measurement will leave the
system.

3 However, once E is measured and, say, the value E_9 is found, then one knows with absolute certainty that the state of the system immediately after this measurement is φ_9.

2· The Initial Square Wave

As a second illustrative example, we consider the following free-particle problem in one dimension. Suppose that at $t = 0$ the system is in the state (Fig. 5.4)

to Consider as probable

(5.24)
$$\psi(x, 0) \begin{cases} \sqrt{\dfrac{1}{L}} & |x| < \dfrac{L}{2} \\ 0 & \text{elsewhere} \end{cases}$$

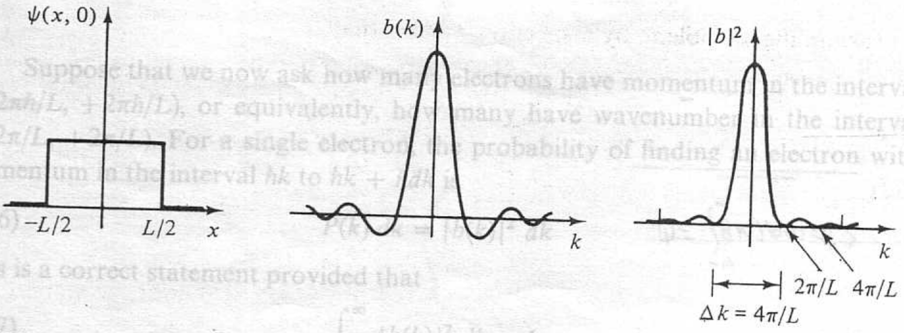


FIGURE 5.4 Square wave packet at $t = 0$ and corresponding momentum eigenstate amplitudes $b(k)$. The interval over which momentum values are most likely to be found is $\Delta p = \hbar\,\Delta k = 4\pi\hbar/L$.

1 If at this same instant, the momentum of the particle is measured, what are the possible values that will be found, and with what probability will these values occur?

† 2 To answer these questions we must first expand $\psi(x, 0)$ in a superposition of the eigenstates of $\hat{p}$:

(5.25)
$$\varphi_k = \frac{1}{\sqrt{2\pi}} e^{ikx}$$

2. Since these states comprise a continuum, the corresponding superposition of eigenstates of $\hat{p}$ is an integral.

(5.26)
$$\psi(x, 0) = \int_{-\infty}^{\infty} b(k)\varphi_k \, dk$$ general definition

3 Inverting this equation (see Eq. 4.42 et seq.) gives the coefficient $b(k)$.

(5.27)
$$\begin{aligned} b(k) &= \int_{-\infty}^{\infty} \psi(x, 0)\varphi_k{}^* \, dx = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(x, 0) e^{-ikx} \, dx \\ &= \frac{1}{\sqrt{2\pi L}} \int_{-L/2}^{+L/2} e^{-ikx} \, dx = \frac{1}{\sqrt{2\pi L}} \frac{2}{k} \left(\frac{e^{ikL/2} - e^{-ikL/2}}{2i} \right) \\ &= \sqrt{\frac{2}{\pi L}} \frac{\sin(kL/2)}{k} \end{aligned}$$

† 3. Again, this coefficient is the projection of the state $\psi(x, 0)$ onto the eigenstate φ_k. Its square times the differential dk is the probability that measurement of momentum yields $p = \hbar k$, in the interval $\hbar k$, $\hbar(k + dk)$. The corresponding probability density (in momentum space) is

(5.28)
$$|b|^2 = \frac{2}{\pi L} \frac{\sin^2(kL/2)}{k^2}$$

This function has its maximum at $k = 0$. It drops to zero at

expand the $\sin\left(\frac{kL}{2}\right)$

$$\frac{kL}{2} = \pi \tag{5.29}$$

or equivalently at

$$p = \hbar k = \frac{2\pi\hbar}{L} \tag{5.30}$$

$x \in \left[-\frac{L}{2}, \frac{L}{2}\right]$, not $x \in [0, L]$

$\to k\left(\frac{L}{2}\right) = \pm n\pi \to k = \frac{2n\pi}{L}$

It is most probable that measurement of momentum finds the value $p = 0$. The momentum values ($\pm n2\pi\hbar/L$) with n an integer greater than 1 are never found, for at these values, $b(k) = 0$.

Referring to Fig. 5.4, we see that the interval of momentum values that measurements are most likely to uncover has the approximate width

$$\Delta k = \frac{4\pi}{L} \tag{5.31}$$

$$\Delta p = \hbar\, \Delta k = \frac{4\pi\hbar}{L}$$

On the other hand, from (5.24), it is uniformly probable that measurement of x finds the particle anywhere in the interval $(-L/2, +L/2)$, of width

$$\Delta x = L \tag{5.32}$$

Combining these two latter uncertainties (5.31 and 5.32) gives

$$\Delta x\, \Delta p \simeq \hbar \tag{5.33}$$

The approximation sign is used because of the qualitative manner in which Δp was calculated. The result (5.33) is another example of the Heisenberg uncertainty principle at work.

The Chopped Beam

To further exhibit the significance of the probability density $|b(k)|^2$, we consider the following problem. Suppose that the free-particle system above is composed of N noninteracting electrons. Every electron is in the state $\psi(x, 0)$ given by (5.24). The density ρ (number/length) is related to ψ through

$$\text{number of particles in } dx = \rho\, dx = N|\psi|^2\, dx \tag{5.34}$$

The total number in the whole "beam" is

$$N = \int_{-\infty}^{\infty} \rho(x)\, dx = N \int_{-L/2}^{L/2} |\psi|^2\, dx = N \tag{5.35}$$

† 2 Suppose that we now ask how many electrons have momentum in the interval
$(-2\pi\hbar/L, +2\pi\hbar/L)$, or equivalently, how many have wavenumber in the interval
2. $(-2\pi/L, +2\pi/L)$. For a single electron, the probability of finding an electron with
momentum in the interval $\hbar k$ to $\hbar k + \hbar dk$ is

$$P(k)\,dk = |b(k)|^2\,dk \tag{5.36}$$

$\psi = \int_{-\infty}^{\infty} dk\, |b(k)\varphi_k\rangle$

3 This is a correct statement provided that

$$\int_{-\infty}^{\infty} |b(k)|^2\,dk = 1 \tag{5.37}$$

If this is not the case, one must divide $|b(k)|^2$ in (5.36) by the last integral.

1 For a totality of N electrons in the beam, the number of them that have momentum in the interval $\hbar k$, $\hbar k + \hbar\,dk$ is

$$\boxed{\rho(k)\,dk = N|b(k)|^2\,dk} \tag{5.38}$$

The total number in the whole beam is

$$N = \int_{-\infty}^{\infty} \rho(k)\,dk = N\int_{-\infty}^{\infty} |b(k)|^2\,dk \tag{5.39}$$

1 For the example at hand

$$\begin{aligned}\int_{-\infty}^{\infty} |b(k)|^2\,dk &= \frac{2}{\pi L}\int_{-\infty}^{\infty} \frac{\sin^2(kL/2)}{k^2}\,dk \\ &= \frac{1}{\pi}\int_{-\infty}^{\infty} \frac{\sin^2\eta\,d\eta}{\eta^2} = 1\end{aligned} \tag{5.40}$$

2 The dummy variable $\eta \equiv kL/2$. To return to the original question, the number of electrons ΔN in the beam with momentum in the interval $(-2\pi\hbar/L, +2\pi\hbar/L)$ is given by the integral

$$\begin{aligned}\Delta N &= N\int_{-2\pi/L}^{+2\pi/L} \frac{2}{\pi L}\frac{\sin^2(kL/2)}{k^2}\,dk \\ &= \frac{N}{\pi}\int_{-\pi}^{+\pi} \frac{\sin^2\eta}{\eta^2}\,d\eta = 0.745N\end{aligned} \tag{5.41}$$

Thus, we find a majority of the electrons in this momentum interval.

4. Superposition and Uncertainty

Let us return to the case of a single electron in the state $\psi(x, 0)$ given by (5.24). Suppose at this time, $t = 0$, we measure the electron's momentum. What value do we find? The answer is: (a) the values $p = \pm n2\pi\hbar/L$ are never found; (b) any other

$$\psi(x) = \delta(x-x') = \frac{1}{\sqrt{2\pi}}\int b(k')\, e^{ik'x}\, dk' = \int_{-\infty}^{\infty} |b(k')\, e^{ik'x}\rangle\, dk'$$

$$\int_{-\infty}^{\infty} |b(k')\varphi_{k'}(x)\rangle\, dk' \Rightarrow \langle \varphi_k | \psi \rangle = \frac{1}{2\pi}\int b(k')\, \delta(k-k)\, dk' = b(k)$$

$$= \frac{1}{\sqrt{2\pi}}\int e^{-ikx}\, \delta(x-x')\, dx = \frac{1}{\sqrt{2\pi}}\, e^{-ikx'}$$

value may occur with corresponding probability density $|b(k)|^2$. Let the measurement find the electron to have the momentum 1

$$p = \frac{\pi\hbar}{L} \tag{5.42}$$

Immediately after this measurement, what is the state of the particle? The answer is

$$\psi = \frac{1}{\sqrt{2\pi}} \exp\left(\frac{i\pi x}{L}\right) \tag{5.43}$$

2 The electron is now in the state (5.43). Suppose that we measure the energy of the particle. What value is found? Since this state is also an eigenstate of $\hat{H}$, it is a certainty that measurement yields

$$E = \frac{(\pi\hbar/L)^2}{2m} \tag{5.44}$$

2· The system is still left in the eigenstate (5.43). Suppose that we now measure the position of the particle. What values may occur? The probability density is

$$P = |\psi|^2 = \frac{1}{2\pi} \tag{5.45}$$

3 which is a constant. It is uniformly probable to find the electron anywhere along the whole x axis. The uncertainty in x is $\Delta x = \infty$. For this same state it is certain that measurement of momentum finds the value $\pi\hbar/L$, so that $\Delta p = 0$. Again we find corroborating evidence for the Heisenberg uncertainty principle.

Now we place a uniform array of scintillation detectors along the x axis. One of them scintillates at $x = x'$. What is the state of the electron immediately after measurement? The answer is the eigenstate of the position operator corresponding to the eigenvalue x' (Fig. 5.5). 1

$$\psi = \delta(x - x') \tag{5.46}$$

† 2 Now we measure momentum again. What values can be found? To answer this question, we again call on the superposition recipe: expand ψ in the eigenstates of $\hat{p}$.

$$\psi = \delta(x - x') = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} b(k)e^{ikx}\, dk \tag{5.47}$$

general definition

$$\langle \phi_k | \psi \rangle = b(k) = \frac{1}{\sqrt{2\pi}} \int \delta(x - x')e^{-ikx}\, dx = \frac{1}{\sqrt{2\pi}} e^{-ikx'}$$

2· The corresponding momentum probability density is

$$P(k) = |b(k)|^2 = \frac{1}{2\pi} \tag{5.48}$$

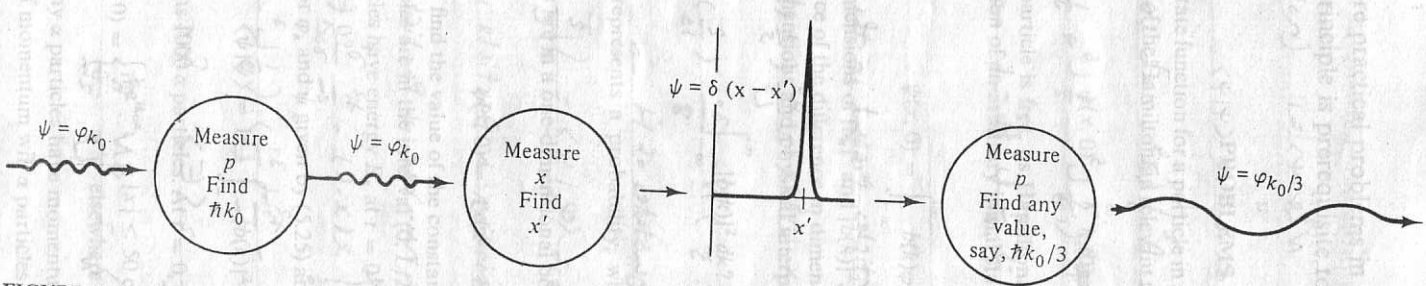


FIGURE 5.5 Measuring x destroys the momentum eigenstate φ_{k_0}.

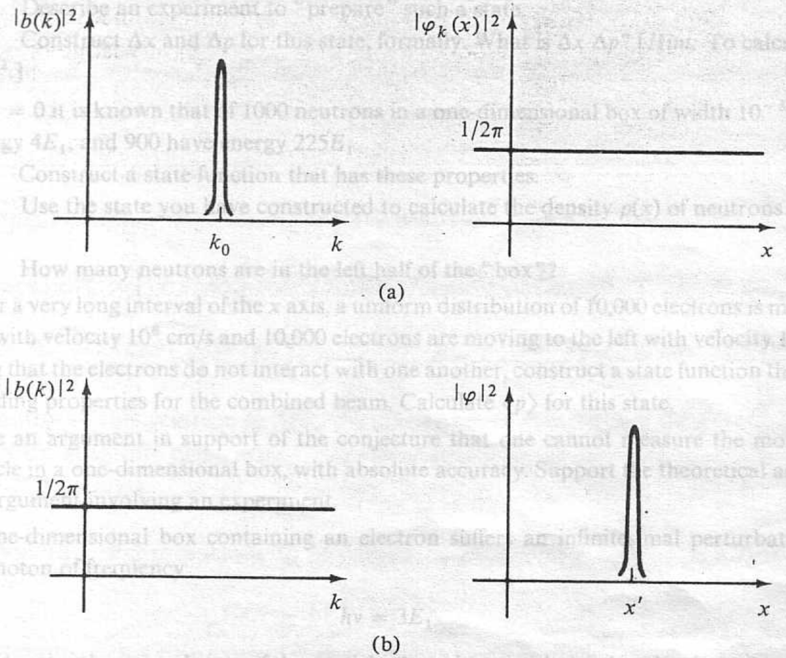


FIGURE 5.6 (a) In the state $\psi = \varphi_{k_0} = (1/\sqrt{2\pi})e^{ik_0x}$, $\Delta p = 0$ and $\Delta x = \infty$. (b) In the state $\psi = \delta(x - x')$, $\Delta x = 0$ and $\Delta p = \infty$.

3 It is uniformly probable to find the electron with any momentum along the whole k axis. The uncertainty in momentum is $\Delta p = \infty$ for the state (5.46), for which $\Delta x = 0$, and the uncertainty principle holds firm (Fig. 5.6).

12 We have been using the phrase superposition principle, but have not given a concise statement of this principle. P. A. M. Dirac, one of the early investigators of quantum mechanics, was first to grasp the full significance of this principle. His
1 description[1] is perhaps the most succinct. The superposition principle "requires us to assume that between . . . states there exist peculiar relationships such that whenever the system is definitely in one state we can consider it as being partly in each of two or more other states. The original state must be regarded as the result of a kind of superposition of the two or more new states, in a way that cannot be conceived on classical ideas."

2 The superposition principle is a cornerstone of quantum mechanics. We have used it previously in some elementary one-dimensional problems. We will return to it in the remainder of the text in relation to more extensive one-dimensional

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[1] P. A. M. Dirac, *The Principles of Quantum Mechanics*, 4th ed., Oxford University Press, New York, 1958.

problems as well as more practical problems in two and three dimensions. A sound understanding of this principle is prerequisite to a working knowledge of quantum mechanics.

PROBLEMS

5.1 If an arbitrary initial state function for a particle in a one-dimensional box is expanded in the discrete series of eigenstates of the Hamiltonian relevant to the box configuration, one obtains (5.6)

$$\psi(x, 0) = \sum_{n=1}^{\infty} b_n(0)\varphi_n(x)$$

On the other hand, if the particle is free, its Hamiltonian has a continuous spectrum of eigenenergies and the superposition of an arbitrary initial state in the eigenstates φ_k of $\hat{H}$ becomes an integral (5.26):

$$\psi(x, 0) = \int_{-\infty}^{\infty} b(k)\varphi_k \, dk$$

(a) What are the dimensions of $|b_n|^2$ and $|b(k)|^2$, respectively?
(b) What is the source of the difference in dimensionality?
(c) What are the dimensions and physical interpretation of the integral

$$\int_{-\infty}^{\infty} |b(k)|^2 \, dk?$$

Answer (partial)

(b) The term $|b_n|^2$ represents a probability, whereas $|b(k)|^2$ represents a probability density.

5.2 One thousand neutrons are in a one-dimensional box, with walls at $x = 0$, $x = L$. At $t = 0$, the state of each particle is

$$\psi(x, 0) = Ax(x - L)$$

(a) Normalize ψ and find the value of the constant A.
(b) How many particles are in the interval $(0, L/2)$ at $t = 0$?
(c) How many particles have energy E_5 at $t = 0$?
(d) What is $\langle E \rangle$ at $t = 0$?

5.3 Using the expressions for φ_k and ψ given by (5.25) and (5.26), respectively, show that

$$\langle \psi | \psi \rangle = 1 \rightarrow \int_{-\infty}^{\infty} |b(k)|^2 \, dk = 1$$

5.4 A pulse 1 m long contains 1000 α particles. At $t = 0$, each α particle is in the state

$$\psi(x, 0) = \begin{cases} \frac{1}{10} e^{ik_0 x}, & |x| \leq 50 \text{ cm}, k_0 = \pi/50 \\ 0 & \text{elsewhere} \end{cases}$$

(a) At $t = 0$, how many α particles have momentum in the interval $(0 < \hbar k < \hbar k_0)$?
(b) At which values of momentum will α particles not be found at $t = 0$?

1 For one particle $\langle\psi|\psi\rangle = 1 \rightarrow$

2 For a 1000-particle $\Psi = N\psi \rightarrow N^2\langle\psi|\psi\rangle = 1$ (not Correct)

$$\rho = N\psi\psi^* \rightarrow N = \int_{xx} \rho\,dx = \underline{N}\langle\psi|\psi\rangle \quad ; \langle\psi|\psi\rangle \not\equiv \psi\psi^*$$

1. $\langle\psi|\psi\rangle = A^2\int_0^L x^2(x-L)^2\,dx = A^2\int_0^L (x^4 - 2x^3L + x^2L^2)\,dx =$

$A^2\left[\frac{1}{5}x^5 - \frac{2L}{4}x^4 + \frac{L^2}{3}x^3\right]_0^L = A^2\left(\frac{1}{5}L^5 - \frac{1}{2}L^5 + \frac{1}{3}L^5\right) = \left(\frac{1}{5}+\frac{1}{3}-\frac{1}{2}\right)L^5A^2 = 1$

$\frac{3}{15}+\frac{5}{15} \Rightarrow \frac{8}{15}-\frac{1}{2} \Rightarrow \frac{16}{30}-\frac{15}{30} \Rightarrow \frac{1}{30}L^5A^2 = 1 \rightarrow A = \sqrt{\frac{30}{L^5}}$

$\psi = \sqrt{\frac{30}{L^5}}\,x(x-L)$.

2. $\rho\,dx$ = Number of particles present in the interval $[x, x+dx]$

$\rightarrow N\int_0^{L/2} \rho\,dx = \frac{30}{L^5}\int_0^{L/2} N x^2(x-L)^2\,dx = \frac{30}{L^5}\left(\frac{1}{5}\left(\frac{L}{2}\right)^5 - \frac{L}{2}\left(\frac{L}{2}\right)^4 + \frac{L^2}{3}\left(\frac{L}{2}\right)^3\right)N$

$= 30\left(\frac{1}{2}\right)^3\left(\frac{1}{20}-\frac{1}{4}+\frac{1}{3}\right)N = \frac{30}{8}\left(\frac{2}{15}\right) = \frac{2\times2}{8}N = \frac{1}{2}N$

3 Expanding ψ in the eigenstates of $\hat{H}$ $\rightarrow$

$$\psi = \sum_{n=1}^{\infty} b_n\varphi_n \rightarrow b_5 = \langle\varphi_5|\psi\rangle = \int\sqrt{\frac{2}{L}}\sin\left(\frac{5\pi x}{L}\right)\sqrt{\frac{30}{L}}(x-L)x\,dx$$

the probability of finding a particle in $\varphi_5 = |b_5|^2 = P(E_5)$

$N|b_5|^2 =$ the most probable number of particle to be fount in φ_5

4 $\langle E\rangle = \langle\psi|\hat{H}|\psi\rangle = \frac{30}{L^5}\int_0^L x(x-L) - \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}(x^2-xL)\,dx =$

$\left(-\frac{\hbar^2}{2m}\right)\frac{30}{L^5}\int_0^L x(x-L)\,dx = -\frac{\hbar^2}{2m}\left(\frac{30}{L^5}\right)\left(\frac{1}{3}L^3-\frac{1}{2}L^3\right) =$

$\frac{\hbar^2}{2m}\frac{30}{L^2}\left(\frac{1}{6}\right) = \frac{5}{L^2}\frac{\hbar^2}{2m} = \langle E\rangle$ for a single particle

For the N particles $\langle E\rangle_N = \frac{5N}{L^2}\frac{\hbar^2}{2m}$

(c) Describe an experiment to "prepare" such a state.

(d) Construct Δx and Δp for this state, formally. What is $\Delta x \, \Delta p$? [*Hint:* To calculate Δp, use $|b(k)|^2$.]

5.5 At $t = 0$ it is known that of 1000 neutrons in a one-dimensional box of width 10^{-5} cm, 100 have energy $4E_1$, and 900 have energy $225E_1$.

(a) Construct a state function that has these properties.

(b) Use the state you have constructed to calculate the density $\rho(x)$ of neutrons per unit length.

(c) How many neutrons are in the left half of the "box"?

5.6 Over a very long interval of the x axis, a uniform distribution of 10,000 electrons is moving to the right with velocity 10^8 cm/s and 10,000 electrons are moving to the left with velocity 10^8 cm/s. Assuming that the electrons do not interact with one another, construct a state function that yields the preceding properties for the combined beam. Calculate $\langle p \rangle$ for this state.

5.7 Give an argument in support of the conjecture that one cannot measure the momentum of a particle in a one-dimensional box, with absolute accuracy. Support the theoretical argument with an argument involving an experiment.

5.8 A one-dimensional box containing an electron suffers an infinitesimal perturbation and emits a photon of frequency

$$h\nu = 3E_1$$

where E_1 denotes the ground state of the particle. A student concludes that the electron was in the state φ_2 prior to perturbation. Is he correct?

Answer

What the student has in mind is that the photon corresponds to the decay

$$h\nu = E_2 - E_1 = 3E_1 .$$

However, suppose that the electron was in the superposition state $(3\varphi_2 + 8\varphi_6)/\sqrt{73}$. Then it is still possible that a photon of frequency $h\nu = 3E_1$ is emitted. So the student is incorrect.

5.9 Measurement of the position of a particle in a one-dimensional box with walls at $x = 0$ and $x = L$ finds the value $x = L/2$.

(a) Show that in subsequent measurement, it is equally probable to find the particle in any odd-energy eigenstate.

(b) Show that the probability of finding the particle in any even-eigenstate is zero. (An eigenstate φ_n is even if n is even and odd if n is odd.)

5.10 It is known that at time $t = 0$, a particle in a box (described in Problem 5.9) is not in the right half of the box. The particle is in one of an infinite number of states. Six such states are depicted in Fig. 5.7.

(a) Write down an approximate wavefunction for each of these states.

(b) Calculate $\langle E \rangle$ for each of these states.

(c) Argue that the state depicted in Fig. 5.7a is the state of minimum $\langle E \rangle$ (assuming that $\varphi = A \sin 2\pi x/L$, $x < L/2$).

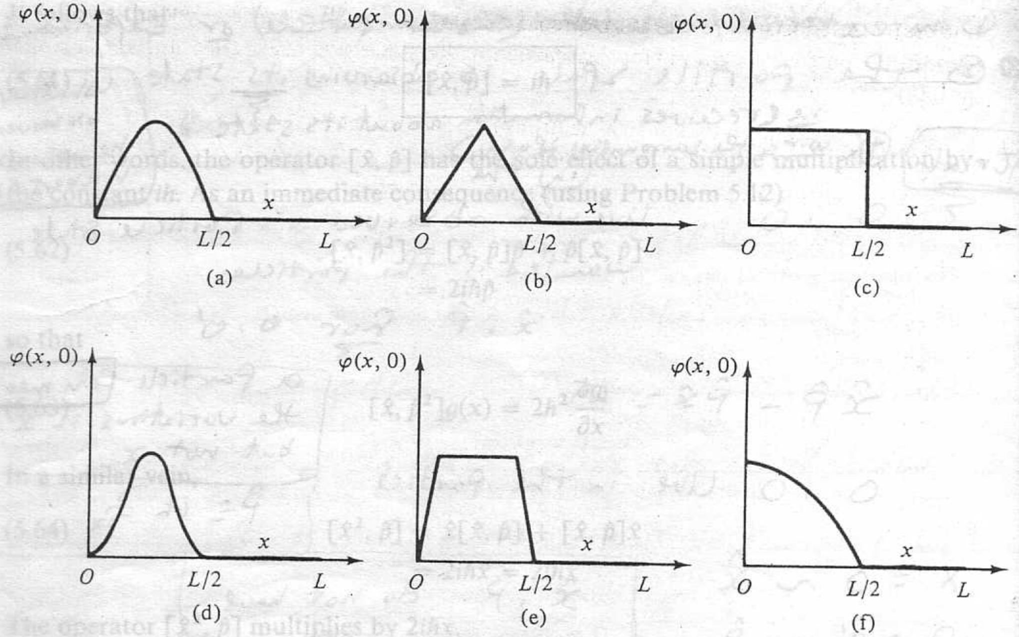

FIGURE 5.7 **Six initial states for a particle in a one-dimensional box, with the property that $|\psi|^2 = 0$ in the right half of the box. (See Problem 5.10.)**

5.11 A particle in the one-dimensional box described in Problem 5.9 is in the ground state. One of the walls of the box is moved to the position $x = 2L$, in a time short compared to the natural period $2\pi/\omega_1$, where $\hbar\omega_1 = E_1$. If the energy of the particle is measured soon after this expansion, what value of energy is most likely to be found? How does this energy compare to the particle's initial energy (E_1)?

5.2 COMMUTATOR RELATIONS IN QUANTUM MECHANICS

An important operation in quantum mechanics is the *commutator* between two operators, $\hat{A}$ and $\hat{B}$. It is written $[\hat{A}, \hat{B}]$ and is defined as

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} \tag{5.49}$$

An immediate property of the commutator is that

$$[\hat{A}, \hat{B}] = -[\hat{B}, \hat{A}] \tag{5.50}$$

If

$$[\hat{A}, \hat{B}] = 0 \tag{5.51}$$

1. Why all the A's can not be measured instantaneously?

i.e → Suppose we have $\hat{A}$ and $\hat{B}$ → Why $\hat{A}$ and $\hat{B}$ can or can not be measured simultaneously?

1. Since there is measurement → we must have eigenvalue eqt^{n}.

Suppose $(\hat{A}\varphi_a = a\varphi_a) \equiv$ measurement of A leaves it in the state φ_a.

But we want to measure A and B → the system is in φ_a,

thus when B is measured → $\hat{B}(\hat{A}\varphi) = a(\hat{B}\varphi_a)$ (1)

[for any A and B, this is not necessarily an eigenvalue eqt^{n}.]

2. How and when (1) becomes exactly representing the simultaneous measurement of $\hat{A}$ and B.

2. Can measurement of A 1st then B differes from B 1st then A?

And if there is a differnce → (i) why there is a difference?

(ii) then, can we still say that A and B are simultaneously measurable?

3. Define simultaneous measurement of A and B?

3. (1) (is either an eigenvalue eqt^{n} or not) is for $t \to 0$ after measurement of A, A is in φ_a → measurement of B either leave the system in φ_a or not?

-1- $\hat{B}(\hat{A}\varphi_a) = a(\hat{B}\varphi_a) = a(\mu\varphi_a)$ → (1) is an eigenvalue eqt^{n}.

-2- $\hat{B}(\hat{A}\varphi_a) = a(\hat{B}\varphi_a)$ → expanding φ_a in the eigenstates of B ⇒ $(\varphi_a \to \psi_B(x,t))$ → $a(\hat{B}\psi_B) = a\lambda\varphi_b)$ → (1) is not an eigenvalue eqt^{n}.

⇒ for 2. → -2- predits that a difference can occur.

And for 2.(ii) $\hat{A}$ and $\hat{B}$ do not shear common eigenf^{ns}.

3 We define simultaneous measurement as:

1) A is not prefered to B ≡ either A or B can be measured 1st → if A is 1st ⇒ $\hat{A}\varphi_a = a\varphi_a$)

2) (Immediately after measurement of A) ≡ (after $0 \le t \to 0$) we measure B.

3) (1) is an eigenvalue eqt^n ≡ ∃ a least a finite number of eigenfunction that are sheared by both $\hat{A}$ and $\hat{B}$.

[This will lead to degeneracy or non degeneracy]

4 Simultaneous measurement for $\hat{A}$ and $\hat{B}$ requires from 1) and 3) that $(\hat{A}\hat{B}) = \hat{B}\hat{A} = (\hat{A}\hat{B})^\dagger$

i.e $(\hat{A}\hat{B} - \hat{B}\hat{A} = 0) \equiv [\hat{A},\hat{B}] = 0 \Rightarrow (5.78)$ and (5.83)

4. $(\hat{A}\hat{B} \neq \hat{B}\hat{A} \Rightarrow (\hat{A}\hat{B} - \hat{B}\hat{A}) = \hat{C} \neq 0) \equiv$ A and B are not simultaneously measurable.

*5 Our 1st assumptions are:

1) (Measurement of A and B) ≡ $\hat{B}\hat{A}\boxed{(\varphi)} \Rightarrow (1)$

2) 4 → non-degeneracy

degeneracy = not necessarily shear all linear combinations like (5.83), but only and only n-linearly independent eigenstates all correspond to the n-fold degenerate eigenvalue a.

the two operators are said to *commute* (*A* and *B* are *compatible*) with each other.
1 That is,

(5.52) $$(\hat{A}\hat{B}) = \hat{B}\hat{A} = (\hat{A}\hat{B})^{\dagger} = \underline{(\hat{B}\hat{A})^{\dagger}}$$

Any operator $\hat{A}$ commutes with any constant a.

(5.53) $$[\hat{A}, a] = 0$$

(5.54) $$[\hat{A}, a\hat{B}] = [a\hat{A}, \hat{B}] = a[\hat{A}, \hat{B}]$$

1 Any operator $\hat{A}$ commutes with its own square, $\hat{A}^2$.

(5.55) $$[\hat{A}, \hat{A}^2] = (\hat{A}\hat{A}^2 - \hat{A}^2\hat{A}) = (\hat{A}\hat{A}\hat{A} - \hat{A}\hat{A}\hat{A}) = 0$$

The meaning of this relation is that, no matter what $\hat{A}$ is, when $[\hat{A}, \hat{A}^2]$ operates on any function $g(x)$, one gets zero, annhilator

(5.56) $$[\hat{A}, \hat{A}^2]g(x) = 0$$

2 More generally, $\hat{A}$ commutes with any function of $\hat{A}$, $f(\hat{A})$.

(5.57) $$[f(\hat{A}), \hat{A}] = 0$$

As an example of this rule, consider the following commutator involving the momentum operator $\hat{p}$.

(5.58) $$[e^{\hat{p}}, \hat{p}] = \left[\sum_{n=0}^{\infty} \frac{\hat{p}^n}{n!}, \hat{p}\right]$$

$$= \sum \frac{1}{n!}[\hat{p}^n, \hat{p}]$$

$$= [1, \hat{p}] + [\hat{p}, \hat{p}] + \frac{1}{2!}[\hat{p}^2, \hat{p}] + \cdots = 0$$

It follows that

(5.59) $$[e^{\hat{p}}, \hat{p}]g(x) = \left[\exp\left(-\frac{i\hbar\partial}{\partial x}\right), -\frac{i\hbar\partial}{\partial x}\right]g(x) = 0$$

where $g(x)$ represents any function of x.

†3 One of the most important commutators in physics is that between the coordinate, $\hat{x}$, and the momentum, $\hat{p}$. Let us calculate it.

(5.60) $$[\hat{x}, \hat{p}]g(x) = i\hbar\left(-x\frac{\partial}{\partial x} + \frac{\partial}{\partial x}x\right)g(x)$$

$$= i\hbar\left(-x\frac{\partial g}{\partial x} + x\frac{\partial g}{\partial x} + g\right) = i\hbar g(x)$$

Spatial Space and moving Space are incompatible
≡ they are independent degrees of freedom.

It follows that

$$\boxed{[\hat{x}, \hat{p}] = i\hbar} \tag{5.61}$$

In other words, the operator $[\hat{x}, \hat{p}]$ has the sole effect of a simple multiplication by
3 the constant $i\hbar$. As an immediate consequence (using Problem 5.12)

$$\begin{aligned}[\hat{x}, \hat{p}^2] &= [\hat{x}, \hat{p}]\hat{p} + \hat{p}[\hat{x}, \hat{p}] \\ &= 2i\hbar\hat{p}\end{aligned} \tag{5.62}$$

so that

$$[\hat{x}, \hat{p}^2]g(x) = 2\hbar^2 \frac{\partial g}{\partial x} \tag{5.63}$$

In a similar vein,

$$\begin{aligned}[\hat{x}^2, \hat{p}] &= \hat{x}[\hat{x}, \hat{p}] + [\hat{x}, \hat{p}]\hat{x} \\ &= 2i\hbar\hat{x} = 2i\hbar x\end{aligned} \tag{5.64}$$

The operator $[\hat{x}^2, \hat{p}]$ multiplies by $2i\hbar x$.

We now prove an important theorem in quantum mechanics which is related to the commutator between two operators. It states: if $\hat{A}$ and $\hat{B}$ commute

$$[\hat{A}, \hat{B}] = 0 \tag{5.65}$$

then $\hat{A}$ and $\hat{B}$ have a set of nontrivial (i.e., other than a constant) common eigenfunctions. The proof is as follows.

1 Let φ_a be the eigenfunction of $\hat{A}$ that corresponds to the eigenvalue a.

$$\hat{A}\varphi_a = a\varphi_a \tag{5.66}$$

Then

$$\hat{B}\hat{A}\varphi_a = a\hat{B}\varphi_a \tag{5.67}$$

Since $\hat{A}$ and $\hat{B}$ commute, the left-hand side of this last equation may be rewritten

$$\hat{A}(\hat{B}\varphi_a) = a(\hat{B}\varphi_a) \tag{5.68}$$

1 Inspection of this equation reveals that $\hat{B}\varphi_a$ is also an eigenfunction of $\hat{A}$ correspond-
2 ing to the eigenvalue a. If φ_a is the only linearly independent (defined below) eigenfunction of $\hat{A}$ that corresponds to the eigenvalue a, the function $\hat{B}\varphi_a$ can differ from φ_a by, at most, a multiplicative constant μ. That is,

$$\hat{B}\varphi_a = \mu\varphi_a \tag{5.69}$$

* Information transfer (≡ Communication) between the Laws of Physics ((Independent Laws do not Communicate ??))

* $\hat{H}\psi = i\hbar\frac{\partial}{\partial t}\psi$ Schrödinger eqtn and (5.61) ⇒

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\underline{r},t)\right]\psi(\underline{r},t) = [\hat{x},\hat{p}]\frac{\partial}{\partial t}\psi(\underline{r},t)$$

* In the Coordinate Space $\hat{x} = x$, $\hat{p} = -i\hbar\nabla$ ⇒

$[\hat{x},\hat{p}]$ and $\frac{\partial}{\partial t}$ Can be interchanged ⇒

* $$\left\| \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\underline{r},t)\right]\psi(\underline{r},t) = \frac{\partial}{\partial t}[\hat{\underline{r}},\hat{\underline{p}}]\psi(\underline{r},t) \right\|$$

* $$\nabla^2 = \frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}$$

$$[\hat{\underline{r}},\hat{\underline{p}}] = i\hbar\left[-\left(x\frac{\partial}{\partial x}+y\frac{\partial}{\partial y}+z\frac{\partial}{\partial z}\right) + \left(\frac{\partial}{\partial x}x+\frac{\partial}{\partial y}y+\frac{\partial}{\partial z}z\right)\right]$$

* $[\hat{\underline{r}},\hat{\underline{p}}] = i\hbar$ ≡ Constant operation ≠ zero

1. $(\hat{A}\varphi_a = a\varphi_a)$, $(\hat{B}\hat{A})\varphi_a = \hat{B}(a\varphi_a) = a(\hat{B}\varphi_a) = \hat{A}(\hat{B}\varphi_a)$

   $(\hat{A}\hat{B})\varphi_a = \quad = a(\mu\varphi_a)$

2. $(\hat{B}\hat{A})\varphi_a = (\hat{A}\hat{B})\varphi_a = (a\mu)\varphi_a = (\mu a)\varphi_a =$

   $\hat{B}(\hat{A}\varphi_a) = \hat{A}(B\varphi_a) = a(\mu\varphi_a) = \mu(a\varphi_a)$

3. There is no difference between the experimental measurement done by an experimentalist and the relative measurement (evaluation) or Observation done by (a Particle or System) to anoter (Particle or System).

$\overrightarrow{\text{arrow of}}$ transfer of information) $A \underset{②}{\overset{①}{\rightleftarrows}} B$ ① (to observe it) or (for it to observe) ②

4. A particle which has no relative frame of reference, and Observing his x Can never determine x, but Can determine its p. → ($\Delta x = \infty$, $\underline{\Delta p} = 0$) ≡ free particle (≡ wave)

   ↳ $\hat{p}$ (Thu. 11-8-1992 10.00 GMT)

Who is observing the state particle (space)

① an external observer (another particle) or Experimentalist

② the partile space is observing its state i.e (receives information about its state) (+) (w.r.t the surrounding space)

Whatever the observer is he belongs to Hilbert space

trial

O, O' $\boxed{\text{in}}$ the live with observed particle state

wanted is the particles

$\hat{x}, \hat{p}$ for O, O'

$$\hat{x}\hat{p} - \hat{p}\hat{x} = i\hbar$$

a particle $\boxed{\text{can measure}}$ the variations in x but not x

$$\hat{p} = i\hbar \frac{\partial}{\partial x}$$

O, O' live in the particle

$X = O \sim \hat{x}$

$p = O' \sim \hat{p}$

$\hat{x}, \hat{p}$ do not have common eigenf$^{\underline{ns}}$

$\hat{x}\hat{p}$ is one process of operator $\boxed{\text{multiplication}}$

operator action followed by the other operator action

i.e $\hat{p}$ (1st), $\hat{x}$ (2nd)

$\hat{p}\hat{x}$ i.e $\hat{x}$ (1st), $\hat{p}$ (2nd)

action (operator acts i.e reveals information x, p depending on the state it act upon

followed rotation (if there is) from where information is recieved

Subtraction $\hat{x}\hat{p} \boxed{-} \hat{p}\hat{x} = i\hbar$

Comparison

* 1st What 2nd How 3rd Why

* Why: if $[\hat{A}, \hat{B}] = \hat{C} \mapsto \hat{A}, \hat{B}$ dose not have Common eigenf$^{\underline{ns}}$ reason in terms of Physics of φ (what is) and Linear independence of the geometry of the space (measure A = A is left in φ_a))

e)

$\hat{P}^2 + \mu^2 = 0 \rightarrow \hat{P} = \pm i\mu \rightarrow \mu = \hbar \frac{\partial}{\partial x}$

$\hat{P} = -i\hbar \frac{\partial}{\partial x}$, [(+ve) is dicarded, why?]

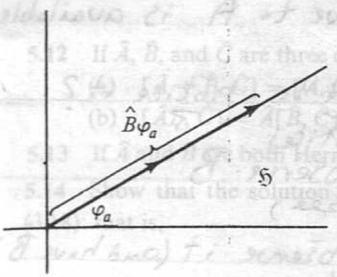

FIGURE 5.8 **If $\hat{B}\varphi_a$ is eigenvector of $\hat{A}$ corresponding to the eigenvalue a, $\hat{B}\varphi_a$ and φ_a are in the same direction in Hilbert space $\mathfrak{H}$.**

2 ($\hat{B}\varphi_a$ and $\mu\varphi_a$ are in the same *direction* in Hilbert space; see Fig. 5.8.) But this is the eigenvalue equation for the operator $\hat{B}$. It follows that φ_a is also an eigenfunction of $\hat{B}$.

2 We have already encountered the implication of this theorem for the problem of the free particle moving in one dimension. For this case

$$[\hat{p}, \hat{H}] = 0 \tag{5.70}$$

It follows by the theorem above that $\hat{p}$ and $\hat{H}$ have common eigenfunctions. They
1 do. We recall that

$$\hat{p}e^{ikx} = \hbar k e^{ikx} \tag{5.71}$$

$$\hat{H}e^{ikx} = \frac{\hbar^2 k^2}{2m} e^{ikx}$$

2 Before pursuing the case when φ_a is not the only linearly independent eigenfunction of $\hat{A}$ corresponding to the eigenvalue a, we consider the definition of linearly independent functions.

Linearly Independent Functions

When is a set of functions a linearly independent set? The N functions of the set $\{\varphi_n\}$ are linearly independent if the linear combination

$$\sum_{n=1}^{N} \lambda_n \varphi_n = 0 \tag{5.72}$$

$x^2 + 1 = 1 + x^2 = 0$

$x^0 + x^2 = 0 \Rightarrow x = \pm i$

$\hat{P} = -i\hbar \frac{\partial}{\partial x} \Rightarrow$

for all x is *only* satisfied when

$$\lambda_1 = \lambda_2 = \cdots = \lambda_n = 0 \tag{5.73}$$

For example, the two functions e^x and $\sin x$ are linearly independent since

$$\lambda_1 e^x + \lambda_2 \sin x = 0 \tag{5.74}$$

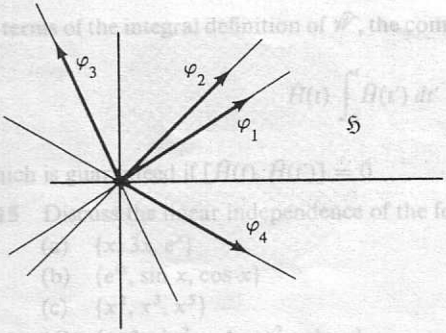

FIGURE 5.9 If $\{\varphi_1, \varphi_2, \varphi_3, \varphi_4\}$ are a linearly independent set, no two lie along the same axis in Hilbert space $\mathfrak{H}$.

for all x is only satisfied by

$$\lambda_1 = \lambda_2 = 0 \tag{5.75}$$

1 The two functions e^x and $3e^x$ are not linearly independent since

$$\lambda_1 e^x + 3\lambda_2 e^x = 0 \tag{5.76}$$

is true for all x if

$$\lambda_1 = -3\lambda_2 \neq 0 \tag{5.77}$$

2 The concept of linearly independent functions has an interesting geometrical interpretation in Hilbert space. If two "vectors" φ_1 and φ_2 in a Hilbert space $\mathfrak{H}$ are linearly independent, they do not lie along the same axis (line) in $\mathfrak{H}$ (Fig. 5.9). Similarly, if the set of N vectors $\{\varphi_n\}$ are linearly independent, no two elements of this set lie on the same axis. If φ_1 and φ_2 are linearly independent, one must "rotate" φ_1 to align it with φ_2. i.e ∃ an angle in $\mathfrak{H}$.

If φ_a is the only linearly independent eigenfunction of $\hat{A}$ corresponding to the eigenvalue a, all eigenfunctions of $\hat{A}$ corresponding to a must be of the form $\mu\varphi_a$. The functions φ_a and $\mu\varphi_a$ are two linearly dependent eigenfunctions of $\hat{A}$ corresponding to the eigenvalue a.

$$\hat{A}(\mu\varphi_a) = \mu\hat{A}\varphi_a = \mu a\varphi_a = a(\mu\varphi_a) \tag{5.78}$$

1 How many such vectors are there? Since μ can be any constant, there is a continuum of such linearly dependent eigenfunctions of $\hat{A}$ corresponding to the eigenvalue a. 2 In any given problem only one of these states is relevant. For bound states ($|\psi|^2 \to 0, |x| \to \infty$), ψ is fixed (and therefore μ) by normalization. For an unbound 2 state ($|\psi|^2 \nrightarrow 0, |x| \to \infty$), ψ is fixed through an appropriate boundary condition. 3 The latter case is appropriate to beam or scattering problems, where the boundary conditions usually involve stipulations on particle current or number density at $|x| = \infty$. These concepts are discussed in greater detail in Section 7.5, which concerns one-dimensional barrier problems.

5 Suppose the fram of referance relative to A is available

is available to A, but A is not able to notice it?

(notice)

then → A dose not have the $\hat{B}$ to Observe B .

(see)

(1) A did not turn to B to observe it (and have $\hat{B}$).

(2) A turned to observe B (but A do not have $\hat{B}$) .

5. Suppow after t, A starts to identify B

and received b => $\hat{B}\phi = b\phi$

(1) If A possesses $\hat{B}$ as a whole; A would have revealed all ϕ_b

(2) How gradually B and all the ϕ_b are received by A?

→ (i) A observes again "for a long time".

(ii) A extrapolates its observation by thinking about B

(iii) A dose not (look) but (think only)
(directly)

(To what extent A is prepared to think about any B)?

Thinking ≡ indirect Observation (watching).

((indirectly))

6 (A loves or is attracted to B but A is not present with B)

((This is the fundamental logical structure of George))

Dose this have any thing to do with Gravity ?

(directly) (do not love)

6. A is present with B, but A is not attracted to B.

presence or non presence of A with B ≡
(absence) ≅

disContinuous presence and its effect on the forces betwen A&B

(1) ⇒ during the absence of B, A thinks about B from the point of view, When A with B $\equiv \Psi_0$

This is a substitute of the force between A and B

(2) during the presence of A with B is there a Continuous interaction (i.e Continuous exchange of information (through Ψ_0), why and why not?

(3) When A is not present with B, what kind of information that is transfered to A other than thinking about B, and how this is related to $\sum_{\neq 0} a\Psi_0$?

7 Reverse the argument to B, Do B think about A

PROBLEMS

5.12 If $\hat{A}$, $\hat{B}$, and $\hat{C}$ are three distinct operators, show that:

(a) $[\hat{A}+\hat{B}, \hat{C}] = [\hat{A}, \hat{C}] + [\hat{B}, \hat{C}]$
(b) $[\hat{A}\hat{B}, \hat{C}] = \hat{A}[\hat{B}, \hat{C}] + [\hat{A}, \hat{C}]\hat{B}$

5.13 If $\hat{A}$ and $\hat{B}$ are both Hermitian, show that $\hat{A}\hat{B}$ is Hermitian if $[\hat{A}, \hat{B}] = 0$.

5.14 Show that the solution to the time-dependent Schrödinger equation given in Problem (3.18): that is,

$$\psi(\mathbf{r}, t) = \exp\left[-\frac{i}{\hbar}\int_0^t dt'\hat{H}(t')\right]\psi(\mathbf{r}, 0)$$

is correct, provided that

$$[\hat{H}(t), \hat{H}(t')] = 0 \qquad (t \neq t')$$

Answer

For $\psi(\mathbf{r}, t)$ as given above to be a solution, the expansion

$$\frac{\partial}{\partial t} e^{\hat{\mathscr{W}}}\psi = e^{\hat{\mathscr{W}}}\frac{\partial \psi}{\partial t} + \underline{e^{\hat{\mathscr{W}}}\hat{H}}\psi$$

must be valid in order to obtain the Schrödinger equation (with $i/\hbar = 1$). For this to be so, $e^{\hat{\mathscr{W}}}$ in the second term must precede $\hat{H}$. Here we have set

$$\hat{\mathscr{W}} \equiv \int_0^t \hat{H}(t')\,dt'$$

We must show that

$$\frac{\partial}{\partial t} e^{\hat{\mathscr{W}}} = e^{\hat{\mathscr{W}}}\frac{\partial \hat{\mathscr{W}}}{\partial t}$$

In general

$$\frac{\partial}{\partial t} e^{\hat{\mathscr{W}}} = \frac{\partial}{\partial t}\left(1 + \hat{\mathscr{W}} + \frac{1}{2}\hat{\mathscr{W}}^2 + \frac{1}{6}\hat{\mathscr{W}}^3 + \cdots\right)$$
$$= \frac{\partial \hat{\mathscr{W}}}{\partial t} + \frac{1}{2}\left(\hat{\mathscr{W}}\frac{\partial \hat{\mathscr{W}}}{\partial t} + \frac{\partial \hat{\mathscr{W}}}{\partial t}\hat{\mathscr{W}}\right) + \cdots$$

Thus the equality above holds if we are able to set

$$\left[\hat{\mathscr{W}}, \frac{\partial \hat{\mathscr{W}}}{\partial t}\right] = 0$$

In this case

$$\frac{\partial}{\partial t} e^{\hat{\mathscr{W}}} = \left(\frac{\partial \hat{\mathscr{W}}}{\partial t} + \hat{\mathscr{W}}\frac{\partial \hat{\mathscr{W}}}{\partial t} + \frac{1}{2}\hat{\mathscr{W}}^2\frac{\partial \hat{\mathscr{W}}}{\partial t} + \cdots\right)$$
$$= e^{\hat{\mathscr{W}}}\frac{\partial \hat{\mathscr{W}}}{\partial t}$$

In terms of the integral definition of $\hat{\mathscr{W}}$, the commutation criterion above becomes

$$\hat{H}(t)\int_0^t \hat{H}(t')\,dt' = \left(\int_0^t \hat{H}(t')\,dt'\right)\hat{H}(t)$$

which is guaranteed if $[\hat{H}(t), \hat{H}(t')] = 0$.

5.15 Discuss the linear independence of the following sets of functions.

(a) $\{x, 3x, e^x\}$
(b) $\{e^{ix}, \sin x, \cos x\}$
(c) $\{x^2, x^3, x^5\}$
(d) $\{x, 3, \sin^2 x, 4\cos^2 x, \ln x\}$

5.16 If μ is an arbitrary constant, the two vectors φ and $\mu\varphi$ in $\mathfrak{H}$ are linearly dependent. Show that the cosine of the angle between these two vectors has modulus 1.

$$|\cos\,\theta| = 1$$

5.17 From Problem 5.16 we conclude that φ and $\mu\varphi$ lie along the same axis in $\mathfrak{H}$. Show also that $\mu\varphi$ is $|\mu|$ times longer than φ, that is, that (see Fig. 5.10)

$$\|\mu\varphi\| = |\mu|\|\varphi\|$$

5.18 Show that if $\hat{A}\varphi_n = a_n\varphi_n$ and $\hat{B}\varphi_n = b_n\varphi_n$ for all eigenvalues $\{a_n\}$ and $\{b_n\}$ of $\hat{A}$ and $\hat{B}$, respectively (i.e., $\hat{A}$ and $\hat{B}$ have completely common eigenstates), then $[A, B] = 0$ on the space of functions spanned by the basis $\{\varphi_n\}$. (*Hint:* Any element of this space may be written

$$\psi = \sum c_n\varphi_n$$

and one need merely show that

$$[\hat{A}, \hat{B}]\sum c_n\varphi_n = 0.)$$

Note: In a more general vein one may say the following: let the eigenstates common to $\hat{A}$ and $\hat{B}$ span a subspace $\mathscr{G}$ of a Hilbert space $\mathfrak{H}$. Then $[\hat{A}, \hat{B}]\psi = 0$, where ψ is any element of $\mathscr{G}$.

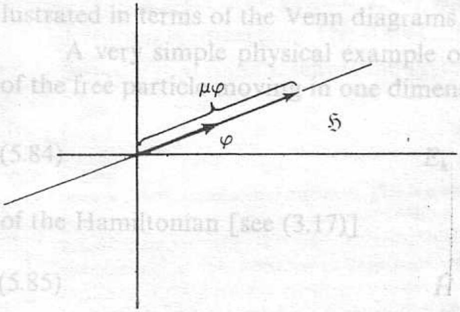

FIGURE 5.10 The vectors φ and $\mu\varphi$ in Hilbert space $\mathfrak{H}$ lie along the same axis and $\|\mu\varphi\| = |\mu|\|\varphi\|$. (See Problem 5.17.)

1. Do the presence of Common eigen states between A and B is necessary for A and B to be Simultaneously measurable? Yes.

Why? go to page (124, 125)' , 5

2. 1- not Commute and shear no Common eigenstates.

2- Commute ($1 \leq n$ degeneracy) →

Shear only n-linearly independent (linear Combination eigenstates) Corresponding to the n-fold degenerate eigenvalue a.

5.3 MORE ON THE COMMUTATOR THEOREM

The Concept of Degeneracy

Suppose there are two (and *only* two) linearly independent eigenfunctions of the operator $\hat{A}$ which both correspond to the eigenvalue a. Call them φ_1 and φ_2.

$$\hat{A}\varphi_1 = a\varphi_1 \qquad (5.79)$$
$$\hat{A}\varphi_2 = a\varphi_2$$

Under such circumstances one says that *the eigenvalue a is doubly degenerate.* The eigenfunctions φ_1 and φ_2 are degenerate. Now we ask, what is the most general eigenfunction of $\hat{A}$ that corresponds to the eigenvalue a? The answer is, any function of the form

$$\varphi_a = \alpha\varphi_1 + \beta\varphi_2 \qquad (5.80)$$

with α and β arbitrary constants. Let us test that this is the case.

$$\hat{A}\varphi_a = \hat{A}(\alpha\varphi_1 + \beta\varphi_2) = \alpha a\varphi_1 + \beta a\varphi_2 \qquad (5.81)$$
$$= a(\alpha\varphi_1 + \beta\varphi_2)$$

In Hilbert space the two functions φ_1 and φ_2 span a plane (two-dimensional subspace). Equation (5.80) indicates that any vector φ_a in this plane is an eigenfunction of $\hat{A}$ corresponding to the eigenvalue a (Fig. 5.11).

Let us return to the commutator theorem discussed in Section 5.2. The operators $\hat{A}$ and $\hat{B}$ commute. If we operate on the first of Eqs. (5.79) with $\hat{B}$ and use the commuting property of $\hat{A}$ and $\hat{B}$, there results

$$\hat{B}\hat{A}\varphi_1 = a(\hat{B}\varphi_1) = \hat{A}(\hat{B}\varphi_1) \qquad (5.82)$$

We conclude that $\hat{B}\varphi_1$ is an eigenstate of $\hat{A}$ that corresponds to the eigenvalue a. But there is a continuum of such eigenstates, all of the form (5.80). All we can say is that there are some α and β such that

$$\hat{B}\varphi_1 = \mu(\alpha\varphi_1 + \beta\varphi_2) \qquad (5.83)$$

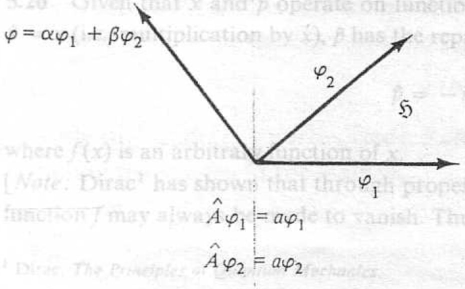
$\varphi = \alpha\varphi_1 + \beta\varphi_2$
φ_2
$\mathfrak{H}$
φ_1
$\hat{A}\varphi_1 = a\varphi_1$
$\hat{A}\varphi_2 = a\varphi_2$

FIGURE 5.11 If φ_1 and φ_2 are two linearly independent degenerate eigenvectors of $\hat{A}$, they span a "plane" (two-dimensional subspace) in Hilbert space $\mathfrak{H}$. Any vector in this plane is an eigenvector of $\hat{A}$ corresponding to the eigenvalue a.

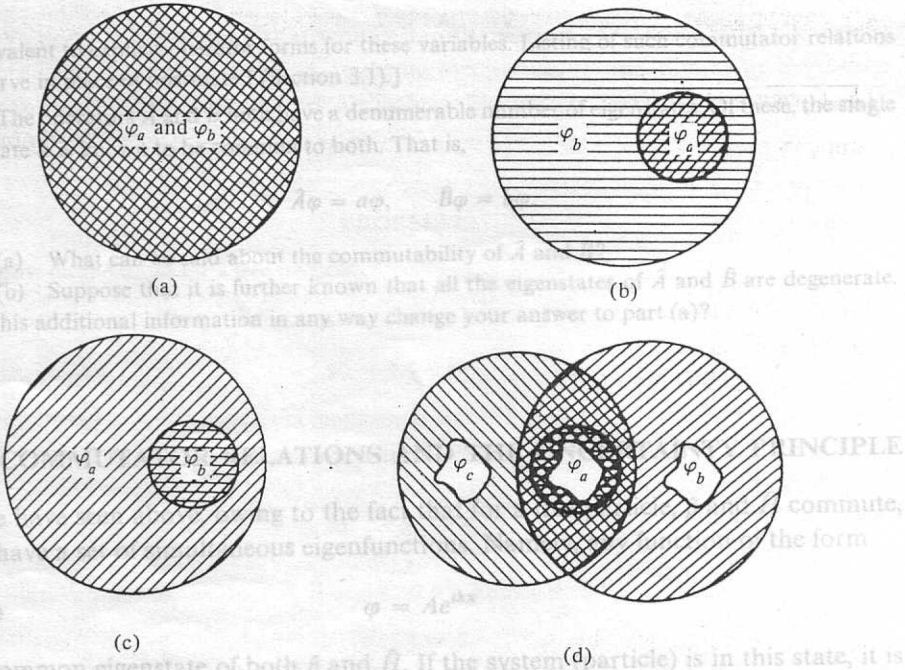

FIGURE 5.12 Various cases pertaining to the sets of eigenfunctions of two compatible operators, $\hat{A}$ and $\hat{B}$. $[\hat{A}, \hat{B}] = 0$. (a) eigenfunctions of $\hat{A}$ = all eigenfunctions of $\hat{B}$. (b) $\hat{A}$ has only nondegenerate eigenfunctions. (c) $\hat{B}$ has only nondegenerate eigenfunctions. (d) $[\hat{A}, \hat{B}] = [\hat{B}, \hat{C}] = [\hat{A}, \hat{C}] = 0$. $\hat{A}$ has only nondegenerate eigenfunctions.

Inspection of this equation [compare with (5.69)] reveals that φ_1 need not be an eigenfunction of $\hat{B}$.

So we have the following rule: If $[\hat{A}, \hat{B}] = 0$, and a is a degenerate eigenvalue of $\hat{A}$, the corresponding eigenfunctions of $\hat{A}$ (which all have the same eigenvalue, a) are not necessarily eigenfunctions of $\hat{B}$. Loosely speaking, degenerate operators have "more" eigenstates than nondegenerate operators. This concept may be illustrated in terms of the Venn diagrams depicted in Fig. 5.12.

A very simple physical example of this situation is provided by the problem of the free particle moving in one dimension. The eigenvalue

$$E_k = \frac{\hbar^2 k^2}{2m} \tag{5.84}$$

of the Hamiltonian [see (3.17)]

$$\hat{H} = \frac{\hat{p}^2}{2m} \tag{5.85}$$

is doubly degenerate. All of the following functions are eigenfunctions of $\hat{H}$ corresponding to this eigenvalue.

$$(\varphi_1, \varphi_2, \varphi_3) = \{(\cos kx, \sin kx, \exp(ikx)\} \tag{5.86}$$

1. This is not a linearly independent set. However, any two are, so that for the free particle the eigenvalue (5.84) is doubly degenerate. For example, the two linearly independent functions, say

$$\{\varphi_1, \varphi_2\} = \{\cos kx, \sin kx\} \tag{5.87}$$

† 2 both have the eigenvalue $\hbar^2k^2/2m$. Although $[\hat{p}, \hat{H}] = 0$, for the free particle, the set of functions (5.87), being degenerate eigenfunctions of energy, need not be eigenfunctions of $\hat{p}$. In fact, they are not.

2. Another linearly independent set of degenerate eigenstates corresponding to the eigenenergy $\hbar^2k^2/2m$ is $\{\varphi_2, \varphi_3\}$. Of these, φ_3 is an eigenstate of $\hat{p}$ and φ_2 is not. Of the set $\{\varphi_1, \varphi_3\}$, φ_1 is not an eigenstate of $\hat{p}$, and again φ_3 is.

3 When there are n (and only n) linearly independent eigenstates of an operator $\hat{A}$ that all correspond to the same eigenvalue, the eigenvalue is *n-fold degenerate*. Suppose that $[\hat{A}, \hat{B}] = 0$. What can then be said is that from these n degenerate eigenstates of $\hat{A}$, one can form n linear combinations which are n linearly independent eigenstates of both $\hat{A}$ and $\hat{B}$.

3. For instance, from the two degenerate eigenstates (5.87) in the free-particle problem above, we can form

$$\varphi_+ = \varphi_1 + i\varphi_2 = \cos kx + i \sin kx = e^{ikx} \tag{5.88}$$

$$\varphi_- = \varphi_1 - i\varphi_2 = \cos kx - i \sin kx = e^{-ikx} \tag{5.89}$$

† These two functions are common eigenstates of $\hat{H}$ and $\hat{p}$. They remain degenerate eigenstates of $\hat{H}$ but are nondegenerate eigenstates of $\hat{p}$.

PROBLEMS

5.19 Construct two linearly independent linear combinations of φ_2 and φ_3 given in (5.87) which are common eigenfunctions of $\hat{H}$ and $\hat{p}$.

5.20 Given that $\hat{x}$ and $\hat{p}$ operate on functions in $\mathfrak{H}_2$ and the relation $[\hat{x}, \hat{p}] = i\hbar$, show that if $\hat{x} = x$ (i.e., multiplication by x), $\hat{p}$ has the representation

$$\hat{p} = -i\hbar \frac{\partial}{\partial x} + f(x)$$

where $f(x)$ is an arbitrary function of x.

[*Note:* Dirac[1] has shown that through proper choice of *phase factor* (Section 4.2), the arbitrary function f may always be made to vanish. Thus, the basic commutator relation between $\hat{x}$ and $\hat{p}$

---

[1] Dirac, *The Principles of Quantum Mechanics*.

is equivalent to explicit operator forms for these variables. Listing of such commutator relations may serve in place of postulate I (Section 3.1).]

5.21 The operators $\hat{A}$ and $\hat{B}$ both have a denumerable number of eigenstates. Of these, the single eigenstate φ is known to be common to both. That is,

$$\hat{A}\varphi = a\varphi, \qquad \hat{B}\varphi = b\varphi.$$

(a) What can be said about the commutability of $\hat{A}$ and $\hat{B}$?

(b) Suppose that it is further known that all the eigenstates of $\hat{A}$ and $\hat{B}$ are degenerate. Does this additional information in any way change your answer to part (a)?

5.4 COMMUTATOR RELATIONS AND THE UNCERTAINTY PRINCIPLE

As we have seen above, owing to the fact that for a free particle, $\hat{p}$ and $\hat{H}$ commute, they have a set of simultaneous eigenfunctions. Namely, any function of the form

$$\varphi = Ae^{ikx} \tag{5.90}$$

is a common eigenstate of both $\hat{p}$ and $\hat{H}$. If the system (particle) is in this state, it is certain that measurement of p gives $\hbar k$ and measurement of energy gives $\hbar^2k^2/2m$. Since (5.90) is a common eigenstate of $\hat{p}$ and $\hat{H}$, measurement of p, which (absolutely) gives $\hbar k$, leaves the particle in the state (5.90). Subsequent measurement of E gives $\hbar^2k^2/2m$ and also leaves the particle in the state (5.90).[1] The operators $\hat{H}$ and $\hat{p}$ are *compatible*; that is, they commute. Quantum mechanics allows p and E to be simultaneously specified (for a free particle). Furthermore, there is only one (unique) state which gives these two values, the state (5.90).

Although there exists a state in which both energy and momentum may be specified simultaneously, the same is not true for the observables $\hat{x}$ and $\hat{p}$. There is no state in which measurement is certain to yield definite values of x and p. Measurement of p leaves the system in an eigenstate of $\hat{p}$ (5.90). Subsequent measurement of x is infinitely uncertain. The state (5.90) is not an eigenstate of $\hat{x}$. Conversely, measurement of x that finds x' leaves the system in the eigenstate of $\hat{x}$,

$$\psi = \delta(x - x') \tag{5.91}$$

---

[1] Here we mean an *ideal* measurement. This is a measurement which *least* perturbs the system. Any real measurement causes the system to suffer a greater perturbation. After the energy of the particle in the state (5.90) is measured, *ideal* measurement maintains that state. However, it is also possible that after finding $\hbar^2k^2/2m$, the particle is in any linear combination of the independent degenerate energy eigenfunctions of $\hat{H}$ which correspond to this eigenvalue (e.g., $\alpha \cos kx + \beta \sin kx$). However, measurement that leaves the particle in this state must have interfered with the momentum, since this state is a superposition of momentum eigenstates. Measurement that leaves the system in the original state (5.90) does not perturb the momentum. It is the *ideal* measurement of energy.

When the particle is in this state, measurement of momentum is infinitely uncertain.

3 For the free particle, there are states in which the uncertainty in energy and momentum obeys the relation

$$\Delta E \Delta p = 0 \tag{5.92}$$

3· On the other hand, in any state, the uncertainties in observation of p and x are such that the product $\Delta p \, \Delta x$ is always greater than a fixed magnitude.

$$\Delta x \, \Delta p \geq \frac{\hbar}{2} \tag{5.93}$$

·2 It is quite clear at this point that these uncertainty relations have their origin in the compatibility properties (5.51) of the operators that correspond to the observables being measured.

1 Suppose that two observables $\hat{A}$ and $\hat{B}$ are not compatible:

$$[\hat{A}, \hat{B}] = \hat{C} \neq 0 \tag{5.94}$$

For example, such is the case for displacement and kinetic energy. Then one can show
2 the following[1]: If measurement of A, in the state ψ, is uncertain by the amount ΔA, then measurement of B is uncertain by the amount ΔB, such that[2]

$$\Delta A \, \Delta B \geq \tfrac{1}{2}|\langle C \rangle| \tag{5.95}$$

2· We recall (Section 3.3) that the uncertainty of an observable A in the state ψ is the root mean square of the deviation of A away from the mean $\langle A \rangle$.

$$(\Delta A)^2 \equiv \langle (A - \langle A \rangle)^2 \rangle = \langle A^2 \rangle - \langle A \rangle^2$$

3 Expectation values in (5.95) are calculated in the state ψ. For example,

$$\langle C \rangle = \langle \psi | \hat{C} \psi \rangle, \qquad (\Delta A)^2 = \langle (\hat{A} - \langle A \rangle)\psi | (\hat{A} - \langle A \rangle)\psi \rangle \tag{5.96}$$

·3 The mechanism at work behind these uncertainty relations is as follows. If $\hat{A}$ †
and $\hat{B}$ do not commute, then the eigenstate φ_a of $\hat{A}$ which the system goes into on
measurement of A is not necessarily an eigenstate of $\hat{B}$. Subsequent measurement
1 of B will give any of the spectrum of eigenvalues of $\hat{B}$ with a corresponding probability
2 distribution $P(b)$. This probability distribution is obtained from the coefficients in the
expansion of φ_a in the eigenstates φ_b of $\hat{B}$.

$$P(b) = \langle \varphi_b | \varphi_a \rangle \tag{5.97}$$

3 (with $\{\varphi_a\}$ and $\{\varphi_b\}$ normalized). Remeasurement of A is then in no way certain of finding the system in the state φ_a.

---

[1] See Problem 5.42.

[2] This generalization of the uncertainty principle is sometimes called the Robertson–Schrödinger relation [H. P. Robertson, *Phys. Rev.* 35, 667A (1930); E. Schrödinger, *Sitzungsber. Preuss. Akad. Wiss.* (1930), p. 296].

We note that the commutator-uncertainty relation, (5.94) and (5.95), is among the more fundamental relations in quantum mechanics. In addition to its important practical significance, it stands as an immutable barrier separating quantum and classical physics.

PROBLEMS

5.22 How do the states for a free particle

$$\varphi_1 = Ae^{ikx}$$

$$\varphi_2 = B\cos kx$$

differ with regard to measurements of momentum and energy?

5.23 For a particle in a one-dimensional potential field $V(x)$, show that

$$\Delta E\,\Delta x \geq \frac{\hbar}{2m}\langle p_x\rangle$$

5.24 Consider three observables, $\hat{A}$, $\hat{B}$, and $\hat{C}$. If it is known that

$$[\hat{B}, \hat{C}] = \hat{A}$$

$$[\hat{A}, \hat{C}] = \hat{B}$$

show that

$$\Delta(AB)\,\Delta C \geq \tfrac{1}{2}\langle A^2 + B^2\rangle$$

5.25 Obtain uncertainty relations for the following products

(a) $\Delta x\,\Delta E$
(b) $\Delta p_x\,\Delta E$
(c) $\Delta x\,\Delta T$
(d) $\Delta p_x\,\Delta T$

relevant to a particle whose kinetic energy is T and whose total energy is E. (A closely related example is discussed in Problem 2.30.)

5.26 If $g(x)$ is an arbitrary function of x, show that

$$[\hat{p}_x, g] = -i\hbar\frac{dg}{dx}$$

5.27 If $g(x)$ and $f(x)$ are both analytic functions, show that

$$g(\hat{A})f(\varphi) = g(a)f(\varphi), \qquad \text{where } \hat{A}\varphi = a\varphi$$

5.28 The time-dependent Schrödinger equation permits the identification

$$\hat{E} = i\hbar\frac{\partial}{\partial t}$$

Using this identification together with the rule (5.95), give a formal derivation of the uncertainty relation

$$\Delta E\,\Delta t \geq \tfrac{1}{2}\hbar$$

Note that in a stationary state (eigenstate of $\hat{H}$), $\Delta E = 0$. The implication for this case is that a stationary state may last indefinitely.

5.29 Can the total energy and linear momentum of a particle moving in one dimension in a constant potential field be measured consecutively with no uncertainty in the values obtained?

5.30 If

$$[\hat{A}, \hat{B}] = i\hat{C}$$

and $\hat{A}$ and $\hat{B}$ are both Hermitian, show that $\hat{C}$ is also Hermitian.

5.31 Prove that if $\hat{A}$ and $\hat{B}$ are Hermitian, $[\hat{A}, \hat{B}]$ is Hermitian if and only if $[\hat{A}, \hat{B}] = 0$.

Answer (*partial*)

Set $[\hat{A}, \hat{B}] \equiv \hat{K}$. Then $\hat{K} = -\hat{K}^{\dagger}$. But $\hat{K}^{\dagger} = \hat{K}$, hence $\hat{K} = -\hat{K}$.

5.32 (a) Obtain an uncertainty relation for mass and time from the relativistic mass-energy equivalency formula.

(b) A free neutron has a mean lifetime of $\simeq 10^3$ s. Apply the uncertainty relation found in part (a) to find the uncertainty in the neutron's mass.

Answer (*partial*)

(b) $\Delta m \simeq 10^{-27}$ amu ($M_p \simeq 1$ amu)

5.5 "COMPLETE" SETS OF COMMUTING OBSERVABLES

We have already seen that for the free particle in one dimension, the eigenvalues of $\hat{H}$ are doubly degenerate. The two eigenfunctions of $\hat{H}$ corresponding to the eigenvalue $\hbar^2 k^2/2m$ are $\exp(+ikx)$ and $\exp(-ikx)$. However, once we specify what p is (say $+\hbar k$), in addition to E, then one can say that the system is in one and only one state, $\exp(+ikx)$ (to within a multiplicative constant). Merely prescribing the energy of the particle does not uniquely determine the state of the particle. Further specifying the momentum removes this ambiguity and the state of the particle is uniquely determined.

Suppose that an operator $\hat{A}$ has degenerate eigenvalues. If a is one of these values, specifying a does not uniquely determine which state the system is in. Let $\hat{B}$ be another operator which is compatible with $\hat{A}$. Consider all the eigenstates $\{\varphi_{ab}\}$ which are common to $\hat{A}$ and $\hat{B}$. Of the degenerate eigenstates of $\hat{A}$, only a subset of these are also eigenfunctions of $\hat{B}$. Under such conditions, if we specify the eigenvalue b and the eigenvalue a, then the state that the system can be in is a smaller set than that determined by specification of a alone. Suppose further that there is only one other operator $\hat{C}$ which is compatible with both $\hat{A}$ and $\hat{B}$. Then they all share a set of common eigenstates. Call these states φ_{abc}. Then

$$\begin{aligned} \hat{A}\varphi_{abc} &= a\varphi_{abc} \\ \hat{B}\varphi_{abc} &= b\varphi_{abc} \\ \hat{C}\varphi_{abc} &= c\varphi_{abc} \end{aligned} \tag{5.98}$$

These functions are still a smaller set than the set $\{\varphi_a\}$ or $\{\varphi_{ab}\}$. Indeed, let us consider that φ_{abc} is *uniquely* determined by the values a, b, and c. This means that having measured a, b, and c: (1) Since φ_{abc} is a common eigenstate of $\hat{A}$, $\hat{B}$ and $\hat{C}$, simultaneous measurement (or a succession of three immediately repeated "ideal" measurements) of A, B, and C will definitely find the values a, b, and c. (2) The state φ_{abc} cannot be further resolved by more measurement. This state contains a maximum of information which is permitted by the laws of quantum mechanics. (3) There are no other operators independent of $\hat{A}$, $\hat{B}$, and $\hat{C}$ which are compatible with these. If there were, the state φ_{abc} could be further resolved. An exhaustive set (in the sense that there are no other independent operators compatible with $\hat{A}$, $\hat{B}$, and $\hat{C}$) of commuting operators such as $\hat{A}$, $\hat{B}$, and $\hat{C}$ above, whose common eigenstates are uniquely determined by the eigenvalues a, b, and c and are a basis of Hilbert space, is called a *complete set of commuting operators.*

Maximally Informative States

The values a, b, and c, which may be so specified in the state φ_{abc}, are sometimes referred to as *good quantum numbers.* These are analogous to the generalized coordinates whose values determine the state of a system classically. As discussed in Section 1.1, such classical coordinates are also labeled *good variables.*

Suppose that there are, in all, five independent operators that specify the properties of a system: $\hat{A}$, $\hat{B}$, $\hat{C}$, $\hat{D}$, and $\hat{F}$. Of these, $\hat{A}$, $\hat{B}$, and $\hat{C}$ are compatible with one another and $\hat{D}$ and $\hat{F}$ are compatible. However, these two sets are incompatible with one another, so that, for example,

$$[\hat{A}, \hat{D}] \neq 0 \tag{5.99}$$

One can simultaneously specify either the eigenvalues a, b, and c or the eigenvalues d and f. One cannot, for instance, say that the system is in a state for which measurement of A definitely gives a and measurement of D definitely gives d. For this case there are two sets of states that are maximally informative: $\{\varphi_{abc}\}$ and $\{\varphi_{df}\}$. Suppose that $\hat{A}$ has degenerate eigenvalue a. What is the state of the system after one has measured and found a? The state lies in a subspace of Hilbert space which is spanned by the degenerate eigenfunctions that correspond to a. This subspace $\mathfrak{H}_a$ has dimensionality $\mathcal{N}_a$ (a is an $\mathcal{N}_a$-fold degenerate eigenvalue). After measurement of $\hat{B}$, the state of the system lies in the space $\mathfrak{H}_{ab}$, which is a subspace of $\mathfrak{H}_a$ and is spanned by the eigenfunction common to $\hat{A}$ and $\hat{B}$. This subspace has dimensionality $\mathcal{N}_{ab}$, which is not greater than $\mathcal{N}_a$.

(5.100)
$$\mathcal{N}_{ab} \leq \mathcal{N}_a$$

Subsequent measurement of $\hat{C}$ (mutually compatible with $\hat{A}$ and $\hat{B}$) leaves the state of the system in a space $\mathfrak{H}_{abc}$ that is a subspace of $\mathfrak{H}_{ab}$ and whose dimensionality does not exceed that of $\mathfrak{H}_{ab}$.

(5.101)
$$\mathcal{N}_{abc} \leq \mathcal{N}_{ab}$$

In this manner we can proceed to measure more and more mutually compatible observables. At each step of the way the eigenstate is forced into subspaces of lesser and lesser dimensionality, until finally after the successive measurement of $A, B, C, D, \ldots$ the state of the system is forced into a subspace of dimensionality $N = 1$. This is a space spanned by only one function. It is the eigenstate common to the complete set of observables $(\hat{A}, \hat{B}, \hat{C}, \hat{D}, \ldots)$: namely, $\varphi_{abcd} \ldots$. This state cannot be further resolved by additional measurements. Measurement of any of the observables $(A, B, C, D, \ldots)$ in this state is certain to find the respective values $(a, b, c, d, \ldots)$.

PROBLEMS

5.33 (a) Show that for a particle in a one-dimensional box, in an arbitrary state $\psi(x, 0)$,

$$\langle E \rangle \geq E_1$$

(b) Under what conditions does the equality maintain?

5.34 A free particle at a given instant of time is in the state

$$\psi = \frac{A}{(xk_0)^2 + 4}$$

At this same instant, (ideal) measurement of the energy finds that

$$E = \frac{\hbar^2 {k_0}^2}{2m}$$

The measurement leaves the momentum uncertain. Under such circumstances, what is the state $\tilde{\psi}$ of the particle immediately after measurement?

Answer

Since the momentum is uncertain after measurement, we know that the state is not one of the eigenstates of momentum $\varphi_{\pm k_0}$. Instead, one may say that the state vector lies in a subspace of $\mathfrak{H}$ spanned by the vectors $\cos k_0 x$ and $\sin k_0 x$.

$$\tilde{\psi} = \alpha \cos k_0 x + \beta \sin k_0 x$$

The coefficients α and β are proportional to the projections of ψ on $\cos k_0 x$ and $\sin k_0 x$, respectively. Since

$$\langle \psi | \sin k_0 x \rangle = 0$$

it follows that after measurement, the state of the particle is

$$\psi = \alpha \cos k_0 x$$

5.35 Show that

$$e^{\hat{A}}\hat{B}e^{-\hat{A}} = \hat{B} + [\hat{A}, \hat{B}] + \frac{1}{2!}[\hat{A}, [\hat{A}, \hat{B}]] + \frac{1}{3!}[\hat{A}, [\hat{A}, [\hat{A}, \hat{B}]]] + \cdots$$

(*Hint:* Taylor-series expand $\hat{f}(\eta) \equiv e^{\eta\hat{A}}\hat{B}e^{-\eta\hat{A}}$ about $\eta = 0$. Also note the derivative property of $\hat{f}(\eta)$: $d\hat{f}/d\eta = [\hat{A}, \hat{f}]$.)

5.36 Show that

$$e^{\hat{A}}e^{\hat{B}} = e^{\hat{A}+\hat{B}}e^{(1/2)[\hat{A}, \hat{B}]}$$

given that $\hat{A}$ and $\hat{B}$ each commutes with $[\hat{A}, \hat{B}]$. (*Hint:* First show that $[e^{\eta\hat{A}}, \hat{B}] = \eta e^{\eta\hat{A}}[\hat{A}, \hat{B}]$. Then establish that the derivative of

$$\hat{g}(\eta) \equiv e^{\eta\hat{A}}e^{\eta\hat{B}}e^{-\eta(\hat{A}+\hat{B})}$$

is

$$\frac{d\hat{g}}{d\eta} = \eta[\hat{A}, \hat{B}]\hat{g}$$

and integrate.) Note that for $\beta \ll 1$, one may always write

$$e^{\beta(\hat{A}+\hat{B})} \simeq e^{\beta\hat{A}}e^{\beta\hat{B}}e^{-(1/2)\beta^2[\hat{A}, \hat{B}]}$$

This relation is important in statistical mechanics, where β plays the role of inverse temperature and $\hat{A} + \hat{B}$ is the Hamiltonian.

5.37 The operator $\hat{A}$ has only nondegenerate eigenvectors and eigenvalues, $\{\varphi_n\}$ and $\{a_n\}$. What are the eigenvectors and eigenvalues of the inverse operator, $\hat{A}^{-1}$? Is your answer consistent with the commutator theorem?

5.38 (a) Construct a one-dimensional wave packet that has zero probability density outside a domain of length L at time $t = 0$ and which has average momentum $\langle p \rangle = +\hbar k_0$. That is, it is propagating to the right.

(b) The wave packet collides with a mass m. What is the probability that the mass is deflected to the left with momentum $-hk_0/4\pi$? (Assume that complete momentum exchange occurs simultaneously at $t = 0$. The mass is located at the origin.)

5.39 Show that the expectation of an observable A of a system that is in the superposition state

$$\psi(x, t) = \sum_n b_n \varphi_n e^{i\omega_n t}$$

may be written in the form

$$\langle A \rangle = 2 \sum_{n>l} \sum b_n{}^* b_l \langle n|A|l \rangle \cos(\omega_n - \omega_l)t + \sum_n |b_n|^2 \langle n|A|n \rangle$$

for $\{b_n{}^* b_l\}$ and $\langle n|A|l\rangle$ real. The states $\varphi_n \exp(i\omega_n t)$ are eigenstates of the Hamiltonian of the system. Here we are writing $|n\rangle$ for φ_n.

5.40 What is the average $\langle x \rangle$ and square root of variance Δx for the following probability densities?

(a) $P(x) = A[1 + (x - x_0)^2]^{-1}$

(b) $P(x) = Ax^2 e^{-x^2/2a^2}$

(c) $P(x) = A \sin^2 \left(\dfrac{x - x_0}{\sqrt{2a}} - 8\pi \right) \exp \left\{ - \left[\dfrac{(x - x_0)^2}{2a^2} \right] \right\}$

5.41 (a) Show that for a particle in a one-dimensional box with walls at $(-L/2, L/2)$

$$\Delta p_{\text{min}} = \sqrt{\langle p^2 \rangle_{\text{min}}} = \frac{h}{2L}$$

(b) Show for this same configuration that

$$\Delta x_{\text{max}} = \sqrt{\langle x^2 \rangle_{\text{max}}} = \frac{L}{2\sqrt{3}}$$

(c) In which states are Δp_{min} and Δx_{max} realized?

(d) From part (a) obtain the following momentum uncertainty relation for this configuration:

$$L\,\Delta p \geq \frac{h}{2}$$

5.42 Given that $\hat{A}$ and $\hat{B}$ are Hermitian operators and that

$$[\hat{A}, \hat{B}] = i\hat{C}$$

show that

$$\Delta A\,\Delta B \geq \tfrac{1}{2}|\langle C \rangle|$$

Answer

1 The uncertainties in $\hat{A}$ and $\hat{B}$, when written in terms of the operators

$$\hat{\delta}_A \equiv \hat{A} - \langle A \rangle$$
$$\hat{\delta}_B \equiv \hat{B} - \langle B \rangle$$

2 appear as

$$(\Delta A)^2 = \langle \hat{\delta}_A \psi | \hat{\delta}_A \psi \rangle = \|\hat{\delta}_A \psi\|^2$$

$$(\Delta B)^2 = \|\hat{\delta}_B \psi\|^2$$

3 These expressions may be incorporated into the Schwartz inequality (Problem 4.20). There results

$$\|\hat{\delta}_A\psi\|^2\|\hat{\delta}_B\psi\|^2 \geq |\langle\hat{\delta}_A\psi|\hat{\delta}_B\psi\rangle|^2$$

3.

$$(\Delta A)^2(\Delta B)^2 \geq |\langle\hat{\delta}_A\psi|\hat{\delta}_B\psi\rangle|^2 = |\langle\psi|\hat{\delta}_A\hat{\delta}_B\psi\rangle|^2$$

The latter equality is due to the Hermiticity of $\hat{\delta}_A$. We now recall that any operator can be written
4 as a linear combination of two Hermitian operators:

$$\hat{\delta}_A\hat{\delta}_B = \frac{1}{2}(\hat{\delta}_A\hat{\delta}_B + \hat{\delta}_B\hat{\delta}_A) + \frac{1}{2}[\hat{\delta}_A, \hat{\delta}_B] \equiv \hat{G} + \frac{i}{2}\hat{C}$$

Here we have used the fact that $[\hat{\delta}_A, \hat{\delta}_B] = [\hat{A}, \hat{B}]$. Substituting the expression above into the preceding inequality gives

$$(\Delta A)^2(\Delta B)^2 \geq \left|\left\langle\psi\left|\left(\hat{G} + \frac{i}{2}\hat{C}\right)\psi\right\rangle\right|^2 = \left|\langle G\rangle + \frac{i}{2}\langle C\rangle\right|^2$$

5 Owing to the Hermiticity of $\hat{G}$ and $\hat{C}$, their expectation values are both real. It follows that

$$(\Delta A)^2(\Delta B)^2 \geq |\langle G\rangle|^2 + \tfrac{1}{4}|\langle C\rangle|^2 \geq \tfrac{1}{4}|\langle C\rangle|^2$$

CHAPTER 6

TIME DEVELOPMENT, CONSERVATION THEOREMS, AND PARITY

6.1 *Time Development of State Functions*
6.2 *Time Development of Expectation Values*
6.3 *Conservation of Energy. Linear and Angular Momentum*
6.4 *Conservation of Parity*

In this chapter we pursue the study of time development of the state function in greater generality than we did in our previous discussion in Chapter 3. This description leads naturally to the concept of constants of the motion in quantum mechanics and again to the notion of stationary states. The distortion of a wave packet in time is obtained with the aid of the free-particle propagator. Classical motion of the packet is obtained in the limit $\hbar \to 0$. *The significance to physics of constants of the motion was described in Chapter 1. We now find that such constants stem from related fundamental symmetries in nature. In the two chapters to follow, the principles and mathematical formalism developed to this point are applied to some practical one-dimensional problems.*

6.1 TIME DEVELOPMENT OF STATE FUNCTIONS

The Discrete Case

Let us recall the recipe for solution to the *initial-value problem* in quantum mechanics (Section 3.5). The initial-value problem poses the question: Given the state $\psi(x, 0)$, at time $t = 0$, what is the state at $t > 0$, $\psi(x, t)$? The answer is: Eq. 3.70.

$$\psi(x, t) = \exp\left(\frac{-i\hat{H}t}{\hbar}\right)\psi(x, 0) \tag{6.1}$$

We recall that the exponential operation is written for its series representation,

$$\exp\left(\frac{-i\hat{H}t}{\hbar}\right) = 1 - \frac{i\hat{H}t}{\hbar} - \frac{\hat{H}^2t^2}{2!\hbar^2} + \cdots \tag{6.2}$$

Suppose that this exponential operator operates on an eigenfunction φ_n of $\hat{H}$. Then $\hat{H}$ as it appears in the exponential is simply replaced by E_n; that is,

$$\exp\left(\frac{-i\hat{H}t}{\hbar}\right)\varphi_n = \exp\left(\frac{-iE_nt}{\hbar}\right)\varphi_n \tag{6.3}$$

As an application of this property we consider the problem of a particle in a one-dimensional box with walls at $(0, L)$, which is initially in an eigenstate of the Hamiltonian of this system.

$$\psi_n(x, 0) = \varphi_n(x) \tag{6.4}$$

Then the state at time t is

$$\psi_n(x, t) = \exp\left(\frac{-i\hat{H}t}{\hbar}\right)\varphi_n(x) = e^{-i\omega_nt}\varphi_n(x)$$

$$\begin{gathered} \psi_n(x, t) = e^{-i\omega_nt}\varphi_n(x) \\ \hbar\omega_n = E_n = n^2E_1 \end{gathered} \tag{6.5}$$

As described in Section 3.6, the time-dependent eigenstates, $\psi_n(x, t)$ of $\hat{H}$, are called *stationary states*. We recall a very important property of a stationary state (3.76)—that the expectation of any operator (which does not contain the time explicitly) is constant in a stationary state. As an example of a stationary state, consider the $n = 5$ eigenstate of the problem at hand,

$$\psi_5(x, t) = e^{-i25E_1t/\hbar}\sqrt{\frac{2}{L}}\sin\left(\frac{5\pi x}{L}\right) \tag{6.6}$$

The eigenstate ψ_5 oscillates with the frequency $25E_1/h$. Both real and imaginary parts of $\psi_5(x, t)$ are *standing waves*. The expectation of energy in this state is constant and equal to $25E_1$.

Suppose, on the other hand, that $\psi(x, 0)$ is not an eigenstate of $\hat{H}$. Under such circumstances, to determine the time development of $\psi(x, 0)$ one calls on the superposition principle and writes $\psi(x, 0)$ as a linear superposition of the eigenstates of $\hat{H}$.

$$\begin{gathered} \psi(x, 0) = \sum b_n\varphi_n(x) \\ b_n = \langle\varphi_n|\psi(x, 0)\rangle \end{gathered} \tag{6.7}$$

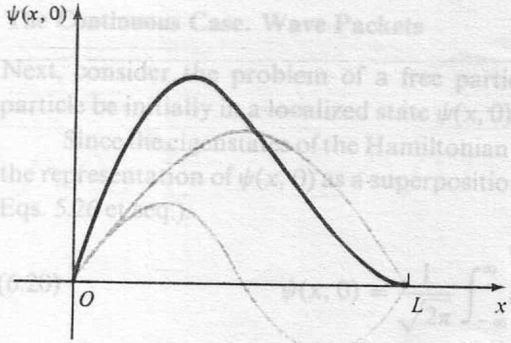

FIGURE 6.1 Initial state

$$\psi(x, 0) = \sqrt{\frac{2}{L}}\left(\frac{\sin(2\pi x/L) + 2\sin(\pi x/L)}{\sqrt{5}}\right)$$

If we now invoke (6.1), the calculation of $\psi(x, t)$ becomes tractable.

$$\begin{aligned} \psi(x, t) &= \exp\left(\frac{-i\hat{H}t}{\hbar}\right)\sum b_n\varphi_n(x) \\ &= \sum b_n \exp\left(\frac{-i\hat{H}t}{\hbar}\right)\varphi_n(x) \qquad (6.8) \\ &= \sum b_n e^{-i\omega_n t}\varphi_n(x) \\ \hbar\omega_n &= E_n = n^2E_1 \end{aligned}$$

This solution indicates that each component amplitude $b_n\varphi_n$ oscillates with the corresponding angular eigenfrequency ω_n.

Consider the specific example in which the initial state is

$$\psi(x, 0) = \sqrt{\frac{2}{L}}\frac{\sin(2\pi x/L) + 2\sin(\pi x/L)}{\sqrt{5}} \tag{6.9}$$

This state is depicted in Fig. 6.1 and is simply the superposition of the two eigenstates φ_2 and φ_1. That is, in the expansion (6.7), one obtains

$$\begin{aligned} b_1 &= \frac{2}{\sqrt{5}}, \qquad b_2 = \frac{1}{\sqrt{5}} \\ b_n &= 0 \qquad \text{(for all other } n\text{)} \end{aligned} \tag{6.10}$$

The state of the system at $t > 0$ is given by (6.8).

$$\psi(x, t) = \sqrt{\frac{2}{L}}\left(\frac{e^{-i\omega_2 t}\sin(2\pi x/L) + 2e^{-i\omega_1 t}\sin(\pi x/L)}{\sqrt{5}}\right) \tag{6.11}$$

How are these time-dependent solutions related to experimental observations? Let us rewrite (6.8) in the form

$$\psi(x, t) = \sum \bar{b}_n(t)\varphi_n(x) \tag{6.12}$$

so that $\bar{b}_n(t)$ now includes the exponential time factor

$$\bar{b}_n(t) \equiv e^{-i\omega_n t} b_n \tag{6.13}$$

Suppose that the energy is measured at $t > 0$. What values will result, and with what probabilities will these values occur? As in Section 5.1, calculation of the expectation of E yields

$$\langle E \rangle = \sum |\bar{b}_n(t)|^2 E_n \tag{6.14}$$

Again, we find that the square of the coefficient of expansion $b_n(t)$ gives the probability that measurement of E at the time t finds the value E_n.

$$P(E_n) = |\bar{b}_n(t)|^2 \tag{6.15}$$

For the state (6.9) this probability distribution is

$$\begin{aligned} P(E_1) &= \tfrac{4}{5} \\ P(E_2) &= \tfrac{1}{5} \\ P(E_n) &= 0 \qquad \text{(for all other } n) \end{aligned} \tag{6.16}$$

For the initial state (6.9), at *any time* $t > 0$, the probability that measurement of energy finds the value E_1 is $\frac{4}{5}$. Similarly, the probability that measurement finds the value $4E_1$ is $\frac{1}{5}$.

What is the expectation of E at $t > 0$ for the initial state (6.9)?

$$\langle E \rangle_{t>0} = \frac{(\langle e^{-i\omega_2 t}\varphi_2| + \langle 2e^{-i\omega_1 t}\varphi_1|)(\hat{H}|e^{-i\omega_2 t}\varphi_2\rangle + \hat{H}|2e^{-i\omega_1 t}\varphi_1\rangle)}{5} \tag{6.17}$$

$$= \frac{E_2 + 4E_1}{5} = \langle E \rangle_{t=0} = \frac{8}{5} E_1$$

The "cross terms" vanish due to orthogonality of the eigenstates of $\hat{H}$, and one finds that the expectation of energy is constant in time. More generally, for any isolated system, in any initial state: (1) the probability of finding a specific energy E_n is constant in time; (2) the expectation $\langle E \rangle$ is constant in time.

These rules follow directly from (6.13)–(6.15).

$$P(E_n) = |\bar{b}_n(t)|^2 = e^{+i\omega_n t} e^{-i\omega_n t} b_n{}^* b_n$$

$$P(E_n) = |b_n|^2 = \text{constant in time} \tag{6.18}$$

$$\langle E \rangle = \sum |b_n(t)|^2 E_n = \sum |b_n|^2 E_n = \text{constant in time} \tag{6.19}$$

The Continuous Case. Wave Packets

Next, consider the problem of a free particle moving in one dimension. Let the particle be initially in a localized state $\psi(x, 0)$ such as that depicted in Fig. 6.2.

Since the eigenstates of the Hamiltonian for a free particle comprise a continuum, the representation of $\psi(x, 0)$ as a superposition of energy eigenstates is an integral (see Eqs. 5.26 et seq.).

$$\psi(x, 0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} b(k) e^{ikx}\, dk \tag{6.20}$$

$$b(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(x, 0) e^{-ikx}\, dx$$

The state of the particle at $t > 0$ follows from (6.1).

$$\psi(x, t) = \exp\left(\frac{-i\hat{H}t}{\hbar}\right) \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} b(k) e^{ikx}\, dk \tag{6.21}$$

$$\psi(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} b(k) e^{i(kx - \omega t)}\, dk$$

$$\hbar\omega = \frac{\hbar^2 k^2}{2m} = E_k \tag{6.22}$$

While the component amplitudes of the state function of a particle in a box oscillate as standing waves, the k-component amplitudes of the free-particle state function propagate. For each value of k, the integrand of (6.22) appears as

$$b(k) \exp\left[ik\left(x - \frac{\omega}{k} t\right)\right] \tag{6.23}$$

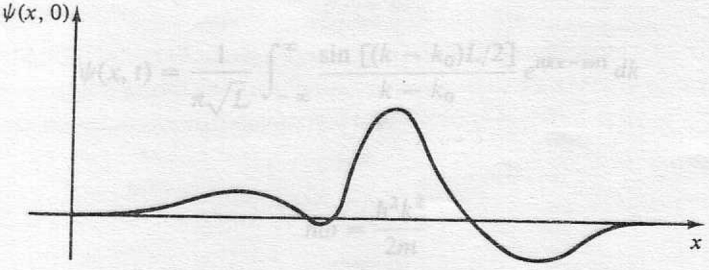

FIGURE 6.2 Initial state for a free particle.

The phase of this component, $[x - (\omega/k)t]$, is constant on the propagating "surface,"

$$x = \frac{\omega}{k}\, t \tag{6.24}$$

This is a surface of constant phase. It propagates with the phase velocity

$$v = \frac{\omega}{k} = \frac{\hbar k}{2m} \tag{6.25}$$

The components with larger wavenumbers (shorter wavelengths) propagate with larger speeds. The long-wavelength components propagate more slowly.

Suppose that at $t = 0$, the state $\psi(x, 0)$ is a tight bundle of eigenstates of $\hat{H}$. When the clocks begin to move, each k-component propagates with a distinct phase velocity. The initial state begins to distort. It may be that the initial state remains somewhat intact and moves. In this case one speaks of a *propagating wave packet*. To have a wave packet propagate, it is necessary that the average momentum of the particle in the initial state does not vanish.

$$\langle p \rangle_{t=0} = \langle \psi(x, 0) | \hat{p} \psi(x, 0) \rangle \neq 0 \tag{6.26}$$

Furthermore, since the packet is localized in space,

$$|\psi(x, 0)|^2 \neq 0 \qquad \text{only over a small domain} \tag{6.27}$$

The velocity with which such a packet moves is called the *group velocity*.

$$v_g = \left. \frac{\partial \omega}{\partial k} \right|_{k_{\max}} \tag{6.28}$$

The meaning of $k_{\max}$ is that the amplitude $|b(k)|^2$ is maximum at $k = k_{\max}$.

$$\hbar k_{\max} \simeq \langle p \rangle = \int_{-\infty}^{\infty} |b(k)|^2 \hbar k \, dk \tag{6.29}$$

This approximation becomes more accurate the more peaked is[1] $|b(k)|^2$.

Combining (6.28) and (6.29) gives

$$\begin{aligned} v_g &= \left. \frac{\partial \omega}{\partial k} \right|_{k\,\max} = \left. \frac{\partial \hbar \omega}{\hbar\, \partial k} \right|_{k\,\max} = \left. \frac{\partial (\hbar^2 k^2/2m)}{\hbar\, \partial k} \right|_{k\,\max} \\ &= \frac{\hbar k_{\max}}{m} = \frac{\langle p \rangle}{m} = v_{CL} \end{aligned} \tag{6.30}$$

The packet moves with the classical velocity $\langle p \rangle / m$.

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[1] However, if $|b(k)|^2$ becomes too peaked, condition (6.27) is violated; that is, $\psi(x)$ spreads out too much.

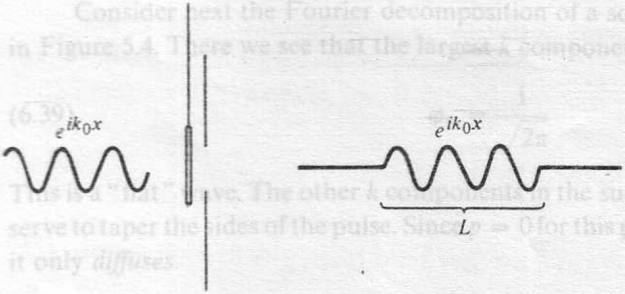

FIGURE 6.3 Chopped wave of length L.

As an example of these concepts, consider a beam of neutrons each of which has momentum $\hbar k_0$. The beam is "chopped," producing a pulse L cm long and containing N neutrons (Fig. 6.3). The state function for each neutron at the instant after the pulse is produced is

$$\psi(x, 0) = \begin{cases} \dfrac{1}{\sqrt{L}} e^{ik_0x} & -\dfrac{L}{2} \le x \le +\dfrac{L}{2} \\ 0 & \text{elsewhere} \end{cases} \tag{6.31}$$

If the momentum of any one of the neutrons is measured at $t > 0$, what values may be found and with what probability do these values occur? To answer this question, we need calculate only the expansion coefficients $b(k)$ of (6.20).

$$\begin{aligned} b(k) &= \frac{1}{\sqrt{2\pi L}} \int_{-L/2}^{+L/2} e^{ik_0x} e^{-ikx}\, dx \\ &= \sqrt{\frac{2}{\pi L}} \frac{\sin[(k - k_0)L/2]}{k - k_0} \end{aligned} \tag{6.32}$$

The state at time $t > 0$ is

$$\psi(x, t) = \frac{1}{\pi\sqrt{L}} \int_{-\infty}^{\infty} \frac{\sin[(k - k_0)L/2]}{k - k_0} e^{i(kx - \omega t)}\, dk \tag{6.33}$$

with

$$\hbar\omega = \frac{\hbar^2 k^2}{2m} \tag{6.34}$$

The amplitude $b(k)$ is sketched in Fig. 6.4.

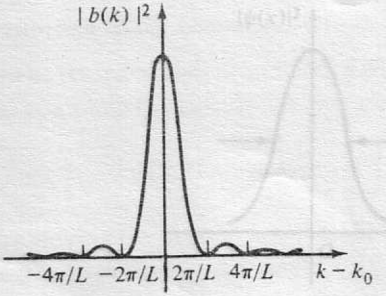

FIGURE 6.4 Momentum probability density corresponding to the pulsed wave of Fig. 6.3.

The momentum probability density $P(k)$ gives the probability that measurement of momentum of any of the neutrons yields a value in the interval $\hbar k$ to $\hbar(k + dk)$. It is given by

$$P(k) = \frac{|b(k)|^2}{\int_{-\infty}^{\infty} |b(k)|^2 \, dk} = |b(k)|^2 \tag{6.35}$$

$$= \frac{2}{\pi L} \frac{\sin^2 [(k - k_0)L/2]}{(k - k_0)^2}$$

This probability density is constant in time.[1] At any time $t > 0$, it is most likely that measurement of momentum of any particle in the pulse finds the value

$$p = \hbar k_{\max} = \hbar k_0 \tag{6.36}$$

Recall that this was the only momentum the neutrons had before the beam was chopped.

At any time $t > 0$, the momentum values

$$\hbar k = \hbar k_0 + \frac{2n\pi\hbar}{L} \qquad (n = 1, 2, 3, \ldots) \tag{6.37}$$

have zero probability of being found. These momentum eigenstates do not enter into the superposition construction of $\psi(x, 0)$.

How many neutrons will be found with momentum in the interval $\hbar(k - k_0) - \hbar k_0$ to $\hbar(k - k_0) + \hbar k_0$? The answer is

$$\Delta N = N \int_{(k - 2k_0)}^{k} |b(k)|^2 \, dk \tag{6.38}$$

This number is also constant in time.

---

[1] This property of the free-particle momentum probability density is more fully developed in Section 7.4.

Consider next the Fourier decomposition of a square wave packet as depicted in Figure 5.4. There we see that the largest k component corresponds to $k = 0$ with

$$\varphi_0 = \frac{1}{\sqrt{2\pi}} \tag{6.39}$$

This is a "flat" wave. The other k components in the superposition of the square wave serve to taper the sides of the pulse. Since $p = 0$ for this packet, it does not propagate—it only *diffuses*.

The Gaussian Wave Packet

A more rewarding problem both from the pedagogical and physical points of view is that of the diffusion and propagation of a *Gaussian wave packet*, discussed previously in Section 3.3. The initial state is

$$\psi(x, 0) = \frac{1}{a^{1/2}(2\pi)^{1/4}} e^{ik_0x} e^{-x^2/4a^2} \tag{6.40}$$

The corresponding initial probability density

$$P(x, 0) = \psi^*\psi = \frac{1}{a\sqrt{2\pi}} e^{-x^2/2a^2} \tag{6.41}$$

is properly normalized as

$$\int_{-\infty}^{\infty} P\, dx = 1$$

The initial uncertainty in position of a particle in the state (6.40) is the square root of the variance

$$\Delta x = a \tag{6.42}$$

The complex modulation $\exp(ik_0x)$ in the state (6.40) serves to give the particle the average momentum

$$\langle p \rangle = \hbar k_0 \tag{6.43}$$

It follows that the initial Gaussian state function (6.40) represents a particle localized within a spread of a about the origin and moving with an average momentum $\hbar k_0$.

The momentum amplitude corresponding to this initial state is

$$\begin{aligned} b(k) &= \frac{1}{a^{1/2}(2\pi)^{3/4}} \int_{-\infty}^{\infty} e^{-x'^2/4a^2} e^{ix'(k_0-k)}\, dx' \\ &= \sqrt{\frac{2a}{\sqrt{2\pi}}}\, e^{-a^2(k_0-k)^2} \end{aligned} \tag{6.44}$$

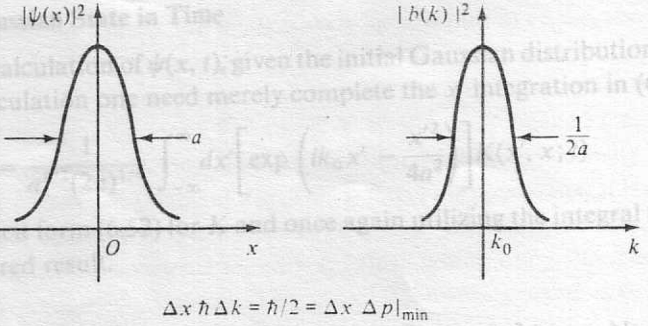

FIGURE 6.5 The momentum probability density $|b|^2$ corresponding to a Gaussian position probability density, $|\psi|^2$, is Gaussian. In this state $\Delta p\, \Delta x$ has its minimum value at $\hbar/2$.

The Fourier transform of a Gaussian is itself Gaussian (see Fig. 6.5). The initial momentum probability density

$$(6.45)\qquad |b(k)|^2 = \frac{2a}{\sqrt{2\pi}} e^{-2a^2(k_0-k)^2}$$

is normalized, centered about the value $k = k_0$, and has a spread $\Delta k = (2a)^{-1}$. It follows that in the initial Gaussian state,

$$(6.46)\qquad \Delta x\, \Delta p\Big|_{\text{Gauss}} = \Delta x \hbar\, \Delta k = \frac{\hbar}{2} = \Delta x\, \Delta p\Big|_{\min}$$

The product of uncertainties has its minimum value in a Gaussian packet.

Free-Particle Propagator

Next we turn to the construction of $\psi(x, t)$ from the initial state (6.40). The value of this function may be obtained from (6.21 et seq.)

$$(6.47)\qquad \psi(x, t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dx'\, dk e^{-ikx'} \psi(x', 0) e^{i(kx-\omega t)}$$

$$= \frac{1}{a^{1/2}} \frac{1}{(2\pi)^{5/4}} \int_{-\infty}^{\infty} dx' \exp\left(ik_0 x' - \frac{x'^2}{4a^2}\right)$$

$$\times \int_{-\infty}^{\infty} dk \exp\left\{i\left[k(x - x') - \frac{k^2a^2t}{\tau}\right]\right\}$$

where the time constant τ is defined as

$$(6.48)\qquad \tau\omega = k^2a^2 \qquad \omega = \frac{\hbar k^2}{2m}$$

Let us take advantage of our construction of $\psi(x, t)$ at this point of the analysis to introduce the free-particle propagator, $K(x', x; t)$. This function provides a formal solution to the free-particle, initial-value problem through the prescription

$$\psi(x, t) = \int_{-\infty}^{\infty} dx' \psi(x', 0) K(x', x; t) \tag{6.49}$$

The explicit form of $K(x', x; t)$ is inferred from (6.47).

$$K(x', x; t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk \exp\left\{ i \left[k(x - x') - \frac{k^2 a^2 t}{\tau} \right] \right\} \tag{6.50}$$

With the aid of the integral (see Problem 6.5)

$$\int_{-\infty}^{\infty} e^{-uy^2} e^{vy}\, dy = \sqrt{\frac{\pi}{u}}\, e^{v^2/4u} \qquad (\operatorname{Re} u > 0) \tag{6.51}$$

there results[1]

$$\begin{aligned} K(x', x; t) &= \sqrt{\frac{\tau}{i4\pi a^2 t}} \exp\left[\frac{i(x - x')^2 \tau}{4a^2 t} \right] \\ &= \sqrt{\frac{m}{2\pi i\hbar t}} \exp\left[\frac{im(x - x')^2}{2\hbar t} \right] \end{aligned} \tag{6.52}$$

Having found this explicit form for the free-particle propagator, let us return to (6.49) and see its meaning. The wavefunction $\psi(x, t)$ gives the probability amplitude related to finding the particle at x at the instant t. If the particle was at x' at $t = 0$, then the probability that it is found at x at $t > 0$ depends on the probability that the particle propagated from x' to x in the interval t. This is what (6.49) says. The probability amplitude that the particle is at x at time t is equal to the initial amplitude that the particle is at x' multiplied by the probability amplitude of propagation from x' to x in the interval t, summed over all x'. Thus we may interpret $K(x, x'; t)$ as the probability amplitude that a particle initially at x' propagates to x in the interval t. It should be noted that the explicit form (6.52) is appropriate only for free-particle propagation. For more general problems involving interaction, the form of (6.49) still maintains, although the propagator function is more complicated (see Problem 6.26).

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[1] To obtain a convergent integral, first replace i by $\alpha \equiv i + \epsilon$, where ϵ is a small real positive number. After integrating, let $\epsilon \to 0$.

Distortion of the Gaussian State in Time

Let us return to the calculation of $\psi(x, t)$, given the initial Gaussian distribution (6.40). To complete the calculation one need merely complete the x' integration in (6.49).

$$\psi(x, t) = \frac{1}{a^{1/2}(2\pi)^{1/4}} \int_{-\infty}^{\infty} dx' \left[\exp\left(ik_0 x' - \frac{x'^2}{4a^2} \right) \right] K(x', x; t)$$

Employing the explicit form (6.52) for K and once again utilizing the integral formula (6.51) gives the desired result.

(6.53)
$$\psi(x, t) = \frac{1}{a^{1/2}(2\pi)^{1/4}(1 + it/\tau)^{1/2}} \exp\left[i \frac{\tau}{t} \left(\frac{x}{2a} \right)^2 \right] \exp\left[- \frac{(i\tau/4a^2 t)(x - \hbar k_0 t/m)^2}{1 + it/\tau} \right]$$

The corresponding probability density is

$$P(x, t) = |\psi(x, t)|^2 = \frac{1}{a\sqrt{2\pi}(1 + t^2/\tau^2)^{1/2}} \exp\left[- \frac{(x - \hbar k_0 t/m)^2}{2a^2(1 + t^2/\tau^2)} \right] \tag{6.54}$$

If we compare this form with the initial probability density we see that the generic shape of $P(x, 0)$ (i.e., that of a bell) has remained intact with three modifications. It has become wider,

$$a \to a(1 + t^2/\tau^2)^{1/2}$$

Second, the center of symmetry of the packet is now at

$$x = v_0 t$$

where we have labeled

$$v_0 \equiv \frac{\hbar k_0}{m}$$

It follows that the probability density of a Gaussian wave packet propagates with a velocity that is directly related to the expectation of momentum of the particle in the Gaussian state. Finally, the height of the density function has diminished.

$$\frac{1}{a\sqrt{2\pi}} \to \frac{1}{a\sqrt{2\pi}(1 + t^2/\tau^2)^{1/2}}$$

The area under the curve P, at any time, remains unity.

A sequence of packet contours is shown in Fig. 6.6. It is quite clear that the packet begins to distort significantly after a time interval τ. If we represent a piece of chalk by a wave packet, $a \simeq 1$ cm, $m \simeq 1$ g, there results

$$\tau \simeq 10^{27} \text{ s} \simeq 10^{20} \text{ yr}$$

But the universe is only $\sim 10^{10}$ yr old. That is why classical objects are never observed to suffer a quantum mechanical spreading.

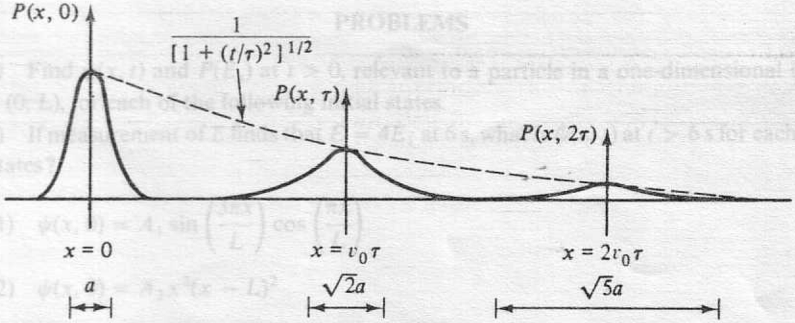


FIGURE 6.6 Shrinkage and spreading of the probability distribution corresponding to a Gaussian wave packet. At any time t,

$$\int_{-\infty}^{\infty} P(x, t)\, dx = 1$$

Flattening of the δ Function

There are two limits that can be taken on the probability density $P(x, t)$ related to the Gaussian wave packet which are very revealing. The first evolves from the initial state

$$P(x, 0) = |\psi(x, 0)|^2 = \delta(x) \tag{6.55}$$

A valid representation of the delta function is given by the limit

$$\delta(x) = \lim_{a \to 0} \frac{1}{a(2\pi)^{1/2}} e^{-x^2/2a^2} \tag{6.56}$$

This function has the correct delta function properties (3.27 et seq.).

Measurement of the position of a particle which finds the value $x = 0$ leaves the particle in the state

$$\psi = \delta(x) \tag{6.57}$$

This state is not normalizable. The state given by (6.55) is a little less sharply peaked than (6.57) and is normalizable.

To obtain the probability density $P(x, t)$ which follows from the initial value (6.55), we merely examine (6.54) in the limit, $a \to 0$. There results

$$\lim P(x, t) = \lim \frac{2ma}{t\hbar\sqrt{2\pi}} \exp\left[-\frac{2a^2(x - \hbar k_0 t/m)^2}{t^2\hbar^2/m^2}\right] \tag{6.58}$$

$$= \lim \frac{2ma}{t\hbar\sqrt{2\pi}} [1 + O(a^2)]$$

The notation $O(a^2)$ denotes "order" of a^2. It stands for a group of terms, the sum of which go to zero like a^2, with decreasing a.

From expression (6.58) we see that for all $t > 0$, P vanishes uniformly for all x, in the limit $a \to 0$. This instantaneous flattening of an infinitely peaked state (6.55) is due to the following circumstance. The momentum probability density $|b(k)|^2$ corresponding to such a state, depicted in Fig. 5.6b, is flat. This means that it is equally probable to find any k value, no matter how large k is, in this state. At any instant $t > 0$, at any point x, the components φ_k with k values which obey the inequality, $(\hbar k/m)t \geq x$, have overtaken that point. The initial infinitely peaked distribution assumes an (almost) instantaneous flattening.[1]

The Classical Particle

The second limit we wish to consider relative to the probability density $P(x, t)$, (6.54), changes $P(x, t)$ to the classical probability relating to a point particle of mass m moving with velocity $\hbar k_0/m$. This is accomplished by setting $\hbar \to 0$ in $P(x, t)$ (except where $\hbar$ appears in $p_0 = \hbar k_0$).

$$\lim_{\hbar \to 0} P(x, t) = \frac{1}{a\sqrt{2\pi}} \exp\left[-\frac{(x - p_0 t/m)^2}{2a^2}\right] \tag{6.59}$$

$$\hbar k_0 = p_0 = \text{constant}$$

For this probability to relate to a "point particle" we impose the additional constraint, $a \to 0$. This gives

$$\lim P(x, t) = \delta\left(x - \frac{p_0 t}{m}\right) = P_{CL}(x, t) \tag{6.60}$$

The probability of finding the particle at t is zero everywhere except on the classical trajectory

$$x = \frac{p_0 t}{m} \tag{6.61}$$

This is another example of the correspondence principle at work. In essence, the "leading term" (i.e., the term not containing $\hbar$) in the expansion of $P(x, t)$ about $\hbar = 0$ gives the classical result.

---

[1] Of course, these conclusions become erroneous for $x/t \geq c$. To obtain a completely physically valid solution for the infinitely peaked initial state, it is necessary to solve the relativistic form of the Schrödinger equation. See related discussions on the *Dirac equation* in A. Messiah, *Quantum Mechanics*, Wiley, New York, 1966.

PROBLEMS

6.1 (a) Find $\psi(x, t)$ and $P(E_n)$ at $t > 0$, relevant to a particle in a one-dimensional box with walls at $(0, L)$, for each of the following initial states.

(b) If measurement of E finds that $E = 4E_1$ at 6 s, what is $\psi(x, t)$ at $t > 6$ s for each of these initial states?

(1) $\psi(x, 0) = A_1 \sin\left(\frac{3\pi x}{L}\right) \cos\left(\frac{\pi x}{L}\right)$

(2) $\psi(x, 0) = A_2 x^2 (x - L)^2$

(3) $\psi(x, 0) = A_3[e^{i\pi(x-L)/L} - 1]$

6.2 Consider the following three dispersion relations.

(1) $\omega^2 = gk$

(2) $\omega^2 = \dfrac{c^2k^2}{1 - (\omega_0/\omega)^2}$

(3) $\omega^2 = {\omega_p}^2 + 3C^2k^2$

The first relation obtains to deep-water surface waves (g is the acceleration due to gravity), the second to electromagnetic waves in a waveguide, and the third to longitudinal waves in a "warm" plasma (ω_p is the *plasma frequency* and C is the *thermal speed*). For all three cases find (1) the phase velocity and (2) the group velocity of a wave packet propagating in the respective medium.

6.3 (a) Show that the free-particle propagator (6.52) has the following property and interpret the result physically.

$$K(x', x; 0) = \delta(x' - x)$$

(b) Show that K satisfies the integral equation

$$K(x', x; t - t_0) = \int K(x', x''; t - t_1) K(x'', x; t_1 - t_0)\, dx''$$

and interpret this result physically in terms of the evolution in time of the state $\psi(x, t_0)$, first from t_0 to t_1 and then from t_1 to t.

Answer (partial)

(a) Set $it = \epsilon^2$ and compare with (C6) of Appendix C. The interpretation of this result is that for infinitesimally short time intervals, the probability amplitude for propagation away from the initial point x' is zero, except in a small neighborhood about the initial point.

6.4 At $t = 0$, 10^5 noninteracting protons are known to be on a line segment 10 cm long. It is equally probable to find any proton at any point on this segment. How many protons remain on the segment at $t = 10$ s? [*Hint*: Let the center of the segment be at $x = 0$. Then the formal answer to the problem with $\psi(x, t)$ normalized is

$$\Delta N = 10^5 \int_{-5}^{5} |\psi(x, 10)|^2\, dx$$

To construct $\psi(x, t)$, the initial square pulse must first be written as a superposition of φ_k states. With $b(k)$ calculated,

$$|\psi(x, t)|^2 = \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dk\, dk' b(k) b^*(k') e^{i(\omega' - \omega)t} e^{i(k - k')x}$$

where ω' is written for $\omega(k')$.]

6.5 The integration involved in obtaining (6.51) is of the type

$$S = \int_{-\infty}^{\infty} e^{-uy^2} e^{vy}\, dy$$

where u and v are constants. Evaluate this integral.

Answer

The aim is to transform the exponent $-uy^2 + vy$ to a perfect square. First we set

$$uy^2 - vy \equiv \alpha^2 y^2 - 2\alpha\beta y$$

which gives

$$\alpha^2 = u, \qquad \beta^2 = \frac{v^2}{4u}$$

The exponent may now be written

$$uy^2 - vy = (\alpha y - \beta)^2 - \beta^2$$

and the integral S becomes (with $\eta = \alpha y - \beta$)

$$S = \frac{e^{\beta^2}}{\alpha} \int_{-\infty}^{\infty} e^{-\eta^2}\, d\eta = \frac{\sqrt{\pi} e^{\beta^2}}{\alpha} = \sqrt{\frac{\pi}{u}}\, e^{v^2/4u}$$

6.6 (a) An electron is in a Gaussian wave packet. If the packet is to remain intact for at least the time it takes light to move across 1 Bohr diameter, $2a_0 = 2\hbar^2/me^2$, what is the minimum width, a, that the Gaussian packet may have (in centimeters)?

(b) What is the diffusion time (τ) for an electron in a Gaussian wave packet of width e^2/mc^2 (in seconds)? This is the classical radius of the electron. How far does light travel in this time (in centimeters)?

6.7 A free particle of mass m moving in one dimension is known to be in the initial state

$$\psi(x, 0) = \sin(k_0 x)$$

(a) What is $\psi(x, t)$?

(b) What value of p will measurement yield at the time t, and with what probabilities will these values occur?

(c) Suppose that p is measured at $t = 3$ s and the value $\hbar k_0$ is found. What is $\psi(x, t)$ at $t > 3$ s?

6.8 A particle moving in one dimension has the wavefunction

$$\psi(x, t) = A \exp [i(ax - bt)]$$

where a and b are constants.

(a) What is the potential field $V(x)$ in which the particle is moving?
(b) If the momentum of the particle is measured, what value is found (in terms of a and b)?
(c) If the energy is measured, what value is found?

(Believe it!) I Love away from my home [Bonny M]

6.2 TIME DEVELOPMENT OF EXPECTATION VALUES

The law that covers the time development of the expectation of an observable, $\langle A \rangle$, follows from the time-dependent Schrödinger equation. We wish to calculate $d\langle A \rangle/dt$.

1 Since $\langle A \rangle$ has all its spatial dependence integrated out, it is at most a function of time. We may therefore write

$$\frac{d\langle A \rangle}{dt} = \frac{\partial \langle A \rangle}{\partial t} \tag{6.62}$$

In the state $\psi(x, t)$, this expression becomes

$$\frac{d\langle \psi | \hat{A}\psi \rangle}{dt} = \int dx \, \frac{\partial}{\partial t} (\psi^* \hat{A} \psi) \tag{6.63}$$

2 The time derivative of the product is

$$\frac{\partial}{\partial t} (\psi^* \hat{A} \psi) = \left(\frac{\partial \psi^*}{\partial t}\right) \hat{A}\psi + \psi^* \hat{A} \frac{\partial \psi}{\partial t} + \psi^* \frac{\partial \hat{A}}{\partial t} \psi \tag{6.64}$$

2· Employing the time-dependent Schrödinger equation

$$\frac{\partial \psi}{\partial t} = \frac{-i\hat{H}}{\hbar} \psi, \qquad \frac{\partial \psi^*}{\partial t} = \frac{i\hat{H}\psi^*}{\hbar} \tag{6.65}$$

in (6.64) gives

$$\frac{\partial}{\partial t} (\psi^* \hat{A} \psi) = \frac{i}{\hbar} \left(\hat{H}\psi^* \hat{A}\psi - \psi^* \hat{A}\hat{H}\psi + \frac{\hbar}{i} \psi^* \frac{\partial \hat{A}}{\partial t} \psi \right) \tag{6.66}$$

Substituting this expansion in (6.63) gives

$$\frac{d\langle \hat{A} \rangle}{dt} = \frac{i}{\hbar} \left(\langle \hat{H}\psi | \hat{A}\psi \rangle - \langle \psi | \hat{A}\hat{H}\psi \rangle + \frac{\hbar}{i} \left\langle \psi \middle| \frac{\partial \hat{A}}{\partial t} \psi \right\rangle \right) \tag{6.67}$$

Since $\hat{H}$ is Hermitian, the first term on the right-hand side of (6.67) may be rewritten to yield the final result,

$$\boxed{\frac{d\langle A\rangle}{dt} = \left\langle \frac{i}{\hbar}[\hat{H}, \hat{A}] + \frac{\partial \hat{A}}{\partial t} \right\rangle} \tag{6.68}$$

If $\hat{A}$ does not contain the time explicitly, then the last term on the right-hand side vanishes and

$$\frac{d\langle A\rangle}{dt} = \frac{i}{\hbar}\langle[\hat{H}, \hat{A}]\rangle \tag{6.69}$$

In the event that $\hat{A}$ commutes with $\hat{H}$, the quantity $\langle A\rangle$ is constant in time and A is called a *constant of the motion*. For a free particle, $\hat{p}$ commutes with $\hat{H}$ and $\langle p\rangle$ is constant in time for any state (wave packet). Since $\hat{H}$ commutes with itself, $\langle H\rangle$, the expectation of the energy, is always constant in time.

-2 Let a particle moving in one dimension be in the presence of the potential $V(x)$. The Hamiltonian of the particle is

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(x) \tag{6.70}$$

How does $\langle x\rangle$ vary in time? Eq. (6.69) gives

$$\begin{aligned} \frac{d\langle x\rangle}{dt} &= \frac{i}{\hbar}\langle[\hat{H}, \hat{x}]\rangle \\ &= \frac{i}{\hbar}\left\langle\left[\frac{\hat{p}^2}{2m}, \hat{x}\right]\right\rangle = \frac{i}{2m\hbar}\langle \hat{p}[\hat{p}, \hat{x}] + [\hat{p}, \hat{x}]\hat{p}\rangle \\ &= \frac{i}{2m\hbar}\langle -2i\hbar p\rangle = \left\langle\frac{p}{m}\right\rangle \end{aligned} \tag{6.71}$$

or, equivalently,

$$m\frac{d\langle x\rangle}{dt} = \langle p\rangle \tag{6.72}$$

This equation bears the same relation between expected values of displacement and momentum as in the classical case. Equation (6.72) cannot hold for the eigenvalues of $\hat{x}$ and $\hat{p}$, since such an equation implies that $x(t)$ and $p(t)$ are simultaneously known.

1. If $\hat{A} \equiv \hat{A}(t)$, therefore, how we see depends on the time in which we looked to measure A, which is time dependent.

2. $[\hat{H}, \hat{p}]\, g(x) = \left(\left(\frac{\hat{p}^2}{2m} + V(x)\right)\hat{p} - \hat{p}\cdot\left(\frac{\hat{p}^2}{2m} + V(x)\right)\right) g(x) =$

$\left(\cancel{\frac{\hat{p}^3}{2m}} - \cancel{\frac{\hat{p}^3}{2m}} + V\hat{p} - \hat{p}V\right) g(x) = -i\hbar\left(V\frac{\partial}{\partial x} g(x) - \frac{\partial}{\partial x}(V g(x))\right)$

$-i\hbar\left[V\cancel{\frac{\partial g}{\partial x}} - V\cancel{\frac{\partial g}{\partial x}} - \frac{\partial V}{\partial x} g\right] = +i\hbar\frac{\partial V}{\partial x} g(x)$

Therefore, $[\hat{H}, \hat{p}] \equiv i\hbar\frac{\partial V}{\partial x} \equiv [\hat{x}, \hat{p}]\frac{\partial V}{\partial x}$

1 For any $\hat{A}$ Can it be a Mathematical (how we see) to ψ the Mathematical

2 To actually (how we measure) depends on $\hat{A}$ and ψ and primarily depends on the design of the measuring apparatus ??

3 Having derived $\hat{A}$, How $\hat{A}$ is related to the design of the measuring apparatus ?

4 How we Can derive mathematically any $\hat{A}$??
reveal

3 Ehrenfest's Principle

The reduction of quantum mechanical equations to classical forms when averages are taken, such as demonstrated above, is known as *Ehrenfest's principle*. Newton's 1 second law follows from the commutator $[\hat{H}, \hat{p}]$, which for the Hamiltonian (6.70) is

$$[\hat{H}, \hat{p}] = i\hbar \frac{\partial V}{\partial x} \tag{6.73}$$

Again using (6.68), one obtains

$$\frac{d\langle p \rangle}{dt} = -\left\langle \frac{\partial V}{\partial x} \right\rangle \tag{6.74}$$

2 which is the x component of the vector relation

$$\frac{d\langle \mathbf{p} \rangle}{dt} = -\langle \nabla V(x, y, z) \rangle = \langle \mathbf{F}(x, y, z) \rangle \tag{6.75}$$

3 where $\mathbf{F}$ is the force at (x, y, z). In any state $\psi(x, t)$, the time development of the averages of $\hat{x}$ and $\hat{p}$ follow the laws of classical dynamics, with the force at any given point replaced by its expectation in the state $\psi(x, t)$.

PROBLEMS

6.9 Show that if $[\hat{H}, \hat{A}] = 0$ and $\partial\hat{A}/\partial t = 0$, then $\langle \Delta A \rangle$ is constant in time.

6.10 Show that

$$\frac{d}{dt}\langle A \rangle = 0$$

in a stationary state, provided that $\partial\hat{A}/\partial t = 0$, using the commutator relation (6.68).

$\equiv H\varphi_n = E_n\varphi_n$

Answer

$$\frac{d\langle A \rangle}{dt} = \frac{i}{\hbar}\langle \varphi_n | [\hat{H}, \hat{A}]\varphi_n \rangle = \frac{i}{\hbar}\langle \varphi_n | (\hat{H}\hat{A} - \hat{A}\hat{H})\varphi_n \rangle$$

$$= \frac{i}{\hbar}(\langle \hat{H}\varphi_n | \hat{A}\varphi_n \rangle - \langle \varphi_n | \hat{A}\hat{H}\varphi_n \rangle)$$

$$= \frac{i}{\hbar}E_n(\langle \varphi_n | \hat{A}\varphi_n \rangle - \langle \varphi_n | \hat{A}\varphi_n \rangle) = 0$$

6.11 Show that for a wave packet propagating in one dimension,

$$m\frac{d\langle x^2 \rangle}{dt} = \langle xp \rangle + \langle px \rangle$$

6.12 A particle moving in one dimension interacts with a potential $V(x)$. In a stationary state of this system show that

$$\tfrac{1}{2}\left\langle x \frac{\partial}{\partial x} V \right\rangle = \langle T \rangle$$

where $T = p^2/2m$ is the kinetic energy of the particle.

Answer

In a stationary state,

(6.74)

$$\underset{?}{\frac{d}{dt}\langle xp \rangle} = \frac{i}{\hbar}\langle [\hat{H}, \hat{x}\hat{p}] \rangle = 0$$

$$\begin{matrix} + \hat{x}\hat{H}\hat{p} \\ - \hat{x}\hat{H}\hat{p} \end{matrix}$$

Expanding the right-hand side, we obtain

$$\begin{aligned} 0 &= \langle \hat{x}[\hat{H}, \hat{p}] + [\hat{H}, \hat{x}]\hat{p} \rangle \\ &= \langle x[\hat{V}, \hat{p}] + [\hat{T}, \hat{x}]\hat{p} \rangle \\ &= i\hbar \left\langle x \frac{\partial V}{\partial x} - 2T \right\rangle \end{aligned}$$

6.13 Consider an operator $\hat{A}$ whose commutator with the Hamiltonian $\hat{H}$ is the constant c.

$$[\hat{H}, \hat{A}] = c$$

Find $\langle A \rangle$ at $t > 0$, given that the system is in a normalized eigenstate of $\hat{A}$ at $t = 0$, corresponding to the eigenvalue a.

6.14 A system is in a superposition of the two energy eigenstates φ_1 and φ_2. Physical properties of the system characteristically depend on the probability density $\psi^*\psi$. Show that resolution of any such property involves measurements over an interval $\Delta t > \hbar/|E_1 - E_2|$.

Answer

The superposition state is

$$\psi(\mathbf{r}, t) = \varphi_1(\mathbf{r}) \exp\left(\frac{-iE_1 t}{\hbar}\right) + \varphi_2(\mathbf{r}) \exp\left(\frac{-iE_2 t}{\hbar}\right)$$

so that

$$\psi^*\psi = |\varphi_1|^2 + |\varphi_2|^2 + 2 \operatorname{Re} \varphi_1{}^*\varphi_2 \exp\left[\frac{i(E_1 - E_2)t}{\hbar}\right]$$

This function oscillates between the two extremes $(|\varphi_1| + |\varphi_2|)^2$ and $(|\varphi_1| - |\varphi_2|)^2$ with the period $\hbar/|E_1 - E_2|$. It follows that changes in related properties become discernible only after an interval greater than or of the same order as this period. The situation is similar to the process of tuning an oscillator to a frequency ω_0 by "listening" for beats. The period between beats varies as the inverse frequency $(\omega - \omega_0)^{-1}$. Thus one is certain that $\omega = \omega_0$ only after an infinite interval.

6.3 CONSERVATION OF ENERGY. LINEAR AND ANGULAR MOMENTUM

The principle of conservation of energy in classical physics states that the energy of an *isolated system* or a *conservative system* is constant in time. A conservative system is one whose dynamics are describable in terms of a potential function. A particle in a one-dimensional box is a conservative system. Suppose that at $t = 0$, the state of the particle is

$$\psi(x, 0) = \frac{3\varphi_1 + 4\varphi_5}{\sqrt{25}} \tag{6.76}$$

What can be said of the energy of the particle at the time $t > 0$? Measurement of the energy has a $\frac{9}{25}$ probability of finding the value E_1 and a $\frac{16}{25}$ probability of finding the value $25E_1$. At $t > 0$ the state (6.76) becomes

$$\psi(x, t) = \frac{3\varphi_1(x)e^{-iE_1t/\hbar} + 4\varphi_5 e^{-E_5t/\hbar}}{\sqrt{25}} \tag{6.77}$$

The probability that measurement yields E_1 is

$$P(E_1) = \frac{(3e^{-iE_1t/\hbar})^*(3e^{-iE_1t/\hbar})}{25} = \frac{9}{25} \tag{6.78}$$

A similar calculation of $P(E_5)$ yields the constant value $\frac{16}{25}$. In other words, in the state given, one cannot say with certainty what the energy is at $t \geq 0$. In what sense is energy conserved? The answer is: in the average sense. It follows directly from (6.69) that

$$\langle H \rangle = \langle E \rangle = \text{constant} \tag{6.79}$$

For the example given, at any instant in time the expectation of the energy is

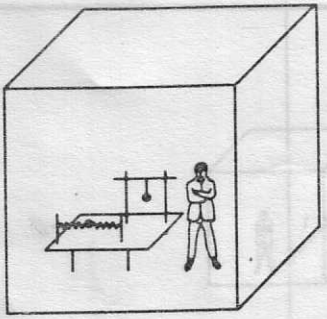
$$\langle E \rangle = \frac{9E_1 + 16E_5}{25} = 16.36E_1 = \text{constant} \tag{6.80}$$

For a free particle, $\hat{p}$ also commutes with $\hat{H}$, hence we can conclude from (6.68) that

$$\langle p \rangle = \text{constant} \tag{6.81}$$

The energy and total momentum of an isolated system are constants of the motion.

Conservation theorems in physics are closely related to symmetry principles. Consider, for example, the fact that the laws of physics do not depend on the time at which they are applied. Newton's second law, Maxwell's equations, and so on, do not change their structure with time. This symmetry of time (i.e., homogeneity) gives rise to the conservation of energy. Let H be the Hamiltonian of the whole universe.



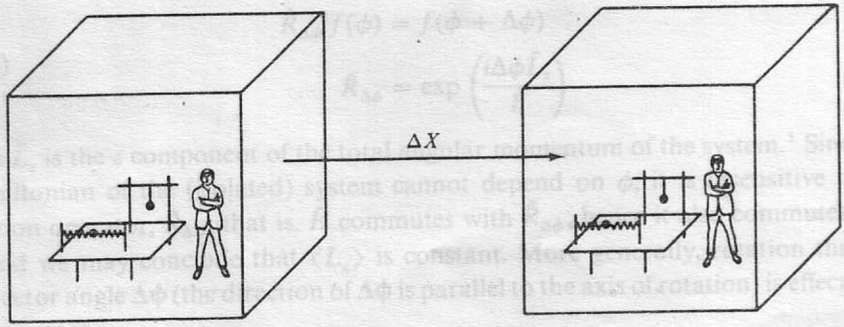
Black box far from any other heavenly bodies

$t = 0, t = t' > 0$

FIGURE 6.7 The laws of physics are the same at t and $t' \rightarrow \partial H/\partial t = 0 \rightarrow \langle E \rangle =$ constant.

3 Homogeneity of time implies that H is not an explicit function of time. This together with (6.68) implies that $d\langle E \rangle/dt = 0$. We may reach the same conclusion for any *isolated system* (Fig. 6.7).

Conservation of momentum for an isolated system depends on the homogeneity of space. Go out in space to a point far removed from other objects. Enclose yourself in a box with no windows and opaque walls. Let the box suffer a "virtual" displacement (Fig. 6.8). There is no experiment which will reveal that the box is at a new location. Consequently, for example, the dynamical laws of an isolated system of particles can only depend on the relative orientation of particles, not on the distances from these particles to some arbitrarily chosen origin. Equivalently, the Hamiltonian of the system can always be transformed so that it does not contain these variables (i.e., the coordinates of the center of mass).



$t = 0$ $t = 0$

FIGURE 6.8 The laws of physics stay the same $\rightarrow \partial H/\partial x = 0 \rightarrow \langle p \rangle =$ constant. Note that in this "thought" experiment, translation occurs in zero time. This is called a "virtual" displacement. It is demanded by the details of the argument. To physically effect a virtual displacement one merely imagines two identical, noninterfering boxes a distance Δx apart.

To find the basis of the relation between the homogeneity of space and conservation of linear momentum, we turn back to Problem 3.17, where it was shown that the $\hat{p}$ operator effects the displacement

$$\hat{\mathscr{D}}(\zeta)f(x) = \exp\left(\frac{i\zeta\hat{p}_x}{\hbar}\right)f(x) = f(x+\zeta) \tag{6.82}$$

In this expression f is any differentiable function of x. For infinitesimal displacement ($\zeta \rightarrow 0$), the displacement operator becomes

$$\hat{\mathscr{D}}(\zeta) = \hat{I} + \frac{i\zeta\hat{p}_x}{\hbar} \tag{6.83}$$

or, equivalently,

$$\hat{p}_x = \frac{\hbar}{i\zeta}[\hat{\mathscr{D}}(\zeta) - \hat{I}]$$

where the identity operator is $\hat{I}$. As observed previously, the Hamiltonian of an isolated system cannot depend on displacement of the system from an origin at an arbitrary point in space. Therefore, the displacement operator $\hat{\mathscr{D}}$ commutes with $\hat{H}$, whence $\hat{p}_x$ does also. Again calling on (6.69), we recapture the constancy of $\langle p_x \rangle$. However, in the present argument we see how this conservation theorem finds its origin in the symmetry of the homogeneity of space. +

In three dimensions the displacement operator becomes

$$\hat{\mathscr{D}}f(\mathbf{r}) = \exp\left(\frac{i\boldsymbol{\zeta}\cdot\hat{\mathbf{p}}}{\hbar}\right)f(\mathbf{r}) = f(\mathbf{r}+\boldsymbol{\zeta}) \tag{6.84}$$

Again, for an isolated system, one may conclude that $\hat{H}$ commutes with $\hat{\mathscr{D}}$ and therefore with $\hat{\mathbf{p}}$, the total linear momentum of the system. It follows that the vector $\langle \mathbf{p} \rangle$ is conserved.

2 Let us return to the experimental "black box" described above. The fact that experiments performed within the box are impervious to the box's location in space or time implies, respectively, conservation of linear momentum and energy. Suppose now that the box undergoes a rotation through the angle $\Delta\phi$ about an arbitrary fixed axis in space. Owing to the isotropy of space, experiments within the box cannot detect such rotational displacement. They are impervious to the box's orientation in space (Fig. 6.9). It follows that the Hamiltonian of the system cannot depend on ϕ, the rotational orientation with respect to some fixed axis, in the same way that it cannot depend on the displacement $\boldsymbol{\zeta}$ from an arbitrary point in space. As a consequence of this rotational symmetry, the total angular momentum of the system is conserved.

Suppose that there is a property of the system which is dependent on the system's rotational orientation ϕ about a fixed axis, which we designate the z axis. Let

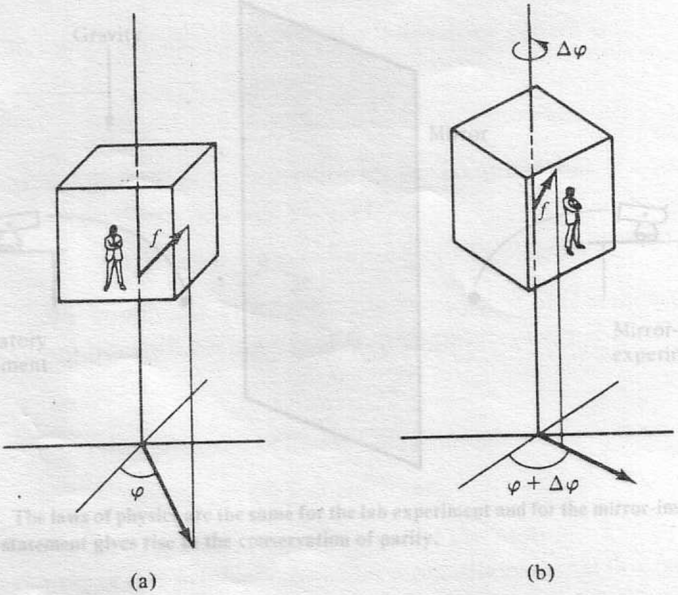


FIGURE 6.9 If $f(\phi)$ is a property of an isolated system that depends on the orientation ϕ of the system about an arbitrary fixed axis, rotation of the system through the angle $\Delta\phi$ causes the property to change to $f(\phi + \Delta\phi)$. Isotropy of space precludes the existence of such a property. This invariance with respect to rotation implies conservation of angular momentum.

the measure of this property be $f(\phi)$. After rotation of the system through the angle $\Delta\phi$, $\phi \rightarrow \phi + \Delta\phi$ and $f(\phi) \rightarrow f(\phi + \Delta\phi)$. This transformation of function is effected by the rotation operator $\hat{R}_{\Delta\phi}$:

$$\hat{R}_{\Delta\phi} f(\phi) = f(\phi + \Delta\phi)$$

$$\hat{R}_{\Delta\phi} = \exp\left(\frac{i\Delta\phi \hat{L}_z}{\hbar}\right) \tag{6.85}$$

Here $\hat{L}_z$ is the z component of the total angular momentum of the system.[1] Since the Hamiltonian of the (isolated) system cannot depend on ϕ, it is insensitive to the rotation operator, $\hat{R}_{\Delta\phi}$; that is, $\hat{H}$ commutes with $\hat{R}_{\Delta\phi}$, hence it also commutes with $\hat{L}_z$ and we may conclude that $\langle L_z \rangle$ is constant. More generally, rotation through the vector angle $\mathbf{\Delta\phi}$ (the direction of $\mathbf{\Delta\phi}$ is parallel to the axis of rotation) is effected by the operator

$$\hat{R}_{\mathbf{\Delta\phi}} = \exp\left(\frac{i\mathbf{\Delta\phi} \cdot \hat{\mathbf{L}}}{\hbar}\right) \tag{6.86}$$

---

[1] This relation is derived in Problem 9.17.

1 Isolated System ~ 2 Conservation Laws (Theorems) ~

Potential function ~ 4 Invariance of the L

rems) ~ 3 System dynamics are describable in terms of a

f the Law Structure ~ 5 Symmetry priciples .

1- f w.r to X in x is f(x)

2- f w.r to X in -x is f(-x)

1. Experiment ≡ f w.r to X is f(x)

2 Mirror Image f w.r to X is f(-x)

3 → f(-x) ≡ the formulation, w.r to X, of the Law obeyed by the image of f in the mirror i.e When x becomes (-1)(x).

The argument demonstrating the constancy of $\hat{L}_z$ carries over to $\hat{\mathbf{L}}$, the total angular momentum of the system.

3 In summary, with $\mathbf{p}$ and $\mathbf{L}$ denoting, respectively, the total linear and angular momentum of an isolated system whose Hamiltonian is H, the following symmetry-conservation principles hold.

Homogeneity of Space

$$[\hat{H}, \hat{\mathbf{p}}] = 0 \rightarrow \frac{d}{dt}\langle \mathbf{p} \rangle = 0 \tag{6.87}$$

Isotropy of Space

$$[\hat{H}, \hat{\mathbf{L}}] = 0 \rightarrow \frac{d}{dt}\langle \mathbf{L} \rangle = 0 \tag{6.88}$$

Homogeneity of Time

$$\frac{\partial \hat{H}}{\partial t} = 0 \rightarrow \frac{d}{dt}\langle E \rangle = 0 \tag{6.89}$$

PROBLEMS

6.15 Under what conditions is the expectation of an operator $\hat{A}$ (which does not contain the time explicitly) constant in time?

Answer

Under either of the following conditions:

(a) $[\hat{A}, \hat{H}] = 0$.

(b) $\langle A \rangle$ is calculated in a stationary state.

6.4 CONSERVATION OF PARITY

Consider an experiment and its mirror image (Fig. 6.10). Such an experiment might be the observation of the orbit of a missile fired in a uniform gravity field, or two particles colliding. These phenomena obey certain physical laws. Suppose that we formulate
1 the laws obeyed by the image orbits in the mirror. They turn out to be the same as the laws that the orbits in the real world obey. This is a symmetry principle. It has no
2 further implication in classical physics. However, in quantum mechanics it is associated with a conservation law, *conservation of parity*.[1]

---

[1] This conservation principle belongs to a class of phenomena called "broken symmetries." Such symmetries are not universally maintained. For example, parity is not conserved in weak-interaction β-decay processes. For further discussion of this topic, see H. Frauenfelder and E. Henley, *Subatomic Physics*, Prentice-Hall, Englewood Cliffs, N.J., 1974.

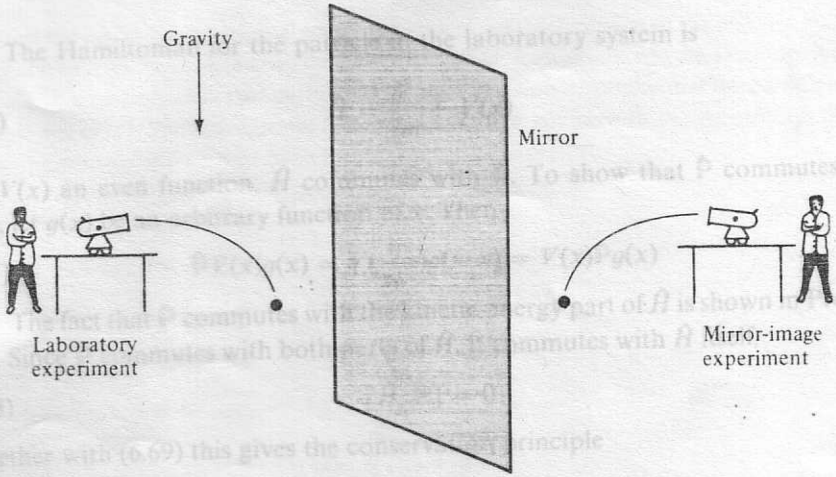


FIGURE 6.10 **The laws of physics are the same for the lab experiment and for the mirror-image experiment. This symmetry statement gives rise to the conservation of parity.**

1 Parity is a property of a function. A function $f(x)$ has *odd parity* if

$$f(-x) = -f(x)$$

A function has *even parity* if (see Fig. 6.11)

$$f(-x) = f(x)$$

1 The parity operator $\hat{\mathbb{P}}$ is defined as[1]

$$\hat{\mathbb{P}}f(x) = f(-x) \tag{6.90}$$

2 What are the eigenvalues of $\hat{\mathbb{P}}$? Let g be an eigenfunction of $\hat{\mathbb{P}}$ with eigenvalue α; then

$$\hat{\mathbb{P}}g(x) = g(-x) = \alpha g(x) \tag{6.91}$$

To find α we operate again with $\hat{\mathbb{P}}$.

$$\hat{\mathbb{P}}\hat{\mathbb{P}}g(x) = \hat{\mathbb{P}}g(-x) = g(x) = \alpha^2 g(x). \tag{6.92}$$

Hence

$$\alpha^2 = 1, \quad \alpha = \pm 1 \tag{6.93}$$

3 For $\alpha = +1$, from (6.91), we obtain

$$g(-x) = g(x) \tag{6.94}$$

---

[1] In three dimensions $\hat{\mathbb{P}}f(x, y, z) = f(-x, -y, -z)$. See Problem 6.23.

Involved, here, are X, $(-1)X \approx \mathbb{P}$, f and $f(x)$

① f w.r to x is available in $f(x)$.

② f w.r to $(-1)x$ is available in $f(-x)$

we have therefore the idea of an operator $\mathbb{P}$ which reverses the observation in X to $(-1)X$

now, w.r to $(-1)x \equiv -x$ f is $f(-x)$

* The idea is : $[\mathbb{P} f(x) = f(-x)] \equiv$ w.r to the $(-1)x$, the $f(x)$ available w.r to x is available in $f(-x)$.

* In Mathematics there is no glass mirrors, all we do is : given the Coordinates of the observer (X), and given the observable f, therefore, we know f at (X) which is received (measured) in $f(x)$

- For my mirror image observer, $-1(X)$, i.e reversed w.r to X, and letting $-1(X) \approx \mathbb{P}$ observe another, but identical, f $\Rightarrow \mathbb{P} f = f(-x) \equiv$ In $-(X)$ w.r to X; let X be G.

* If there observation done by $(-1)X$ is not available, and

α there is no real glass mirror, still we Can understand $\mathbb{P} f$ as X riding over f and looking behind to himself.

The argument demonstrating the constancy of J_z carries over to $\mathbf{L}$, the total angular momentum of the system.

In summary, with $\mathbf{p}$ and $\mathbf{L}$ denoting, respectively, the total linear and angular momentum of an isolated system whose Hamiltonian is $\hat{H}$, the following symmetry conservation principles hold.

Homogeneity of Space

$$[\hat{H}, \hat{\mathbf{p}}] = 0 \to \frac{d}{dt}\langle \hat{\mathbf{p}} \rangle = 0 \tag{6.87}$$

Isotropy of Space

$$[\hat{H}, \hat{\mathbf{L}}] = 0 \to \frac{d}{dt}\langle \hat{\mathbf{L}} \rangle = 0 \tag{6.88}$$

Homogeneity of Time

$$\frac{\partial \hat{H}}{\partial t} = 0 \to \frac{d}{dt}\langle \hat{H} \rangle = 0 \tag{6.89}$$

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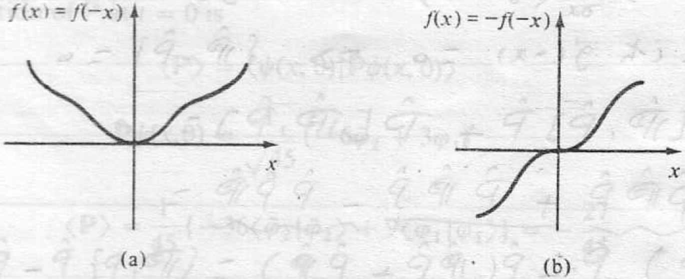

FIGURE 6.11 Any even function is an eigenfunction of $\hat{\mathbb{P}}$ with eigenvalue $+1$:

$$\hat{\mathbb{P}}f(x) = +1f(x)$$

Any odd function is an eigenfunction of $\hat{\mathbb{P}}$ with eigenvalue -1:

$$\hat{\mathbb{P}}f(x) = -1f(x)$$

Any even function is an eigenfunction of $\hat{\mathbb{P}}$ with eigenvalue $+1$. For $\alpha = -1$,

$$g(-x) = -g(x) \tag{6.95}$$

4 Any odd function is an eigenfunction of $\hat{\mathbb{P}}$ with eigenvalue -1. The order of degeneracy † of $\alpha = \pm 1$ is infinite. There are no other eigenvalues of $\hat{\mathbb{P}}$.

-2 How is this parity property connected with the symmetry principle relating to
1 mirror images mentioned above? Consider that a particle (m) moving in one dimension interacts with another stationary particle (M) which is at the position $x = 0$. The
1 potential of interaction between the particles is $V(x)$. Suppose that the (moving)
2 particle is at a position $x' > 0$. The image of the particle seen in a mirror which intersects the x axis normally at $x = 0$ is at $x = -x' < 0$ (Fig. 6.12). The temporal
3 behavior of the image particle will be the same as that for the laboratory particle if $V(x) = V(-x)$. [The potential "seen" by the image particle is $V(-x)$.]

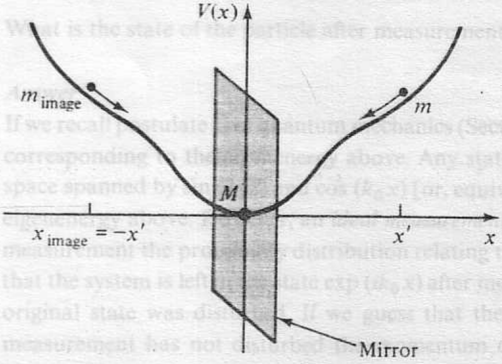

FIGURE 6.12 A mass m interacting with stationary mass M through potential $V(x)$. If image dynamics is to be the same as lab dynamics, $V(x) = V(-x)$.

1. The Hamiltonian for the particle in the laboratory system is

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(x) \tag{6.96}$$

1 For $V(x)$ an even function, $\hat{H}$ commutes with $\hat{\mathbb{P}}$. To show that $\hat{\mathbb{P}}$ commutes with $V(x)$, let $g(x)$ be an arbitrary function of x. Then

$$\hat{\mathbb{P}}V(x)g(x) = V(-x)g(-x) = V(x)\hat{\mathbb{P}}g(x) \tag{6.97}$$

2 The fact that $\hat{\mathbb{P}}$ commutes with the kinetic-energy part of $\hat{H}$ is shown in Problem 6.16. Since $\hat{\mathbb{P}}$ commutes with both parts of $\hat{H}$, it commutes with $\hat{H}$ itself.

$$[\hat{H}, \hat{\mathbb{P}}] = 0 \tag{6.98}$$

3 Together with (6.69) this gives the conservation principle

$$\langle \mathbb{P} \rangle = \text{constant} \tag{6.99}$$

† The parity of the state of a system is a constant of the motion.

As an example of this principle, consider a one-dimensional box centered at the origin, so that its walls are at $x = L/2$, $x = -L/2$ (see Problem 4.1). The eigenstates of the Hamiltonian for this system are

$$\tilde{\varphi}_n = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \quad (n = 2, 4, 6, \ldots, 2j, \ldots) \tag{6.100}$$

$$\varphi_n = \sqrt{\frac{2}{L}} \cos\left(\frac{n\pi x}{L}\right) \quad (n = 1, 3, 5, \ldots, 2j + 1, \ldots)$$

1 The eigenstates $\tilde{\varphi}_n$ are odd while φ_n are even.

$$\begin{aligned} \hat{\mathbb{P}}\tilde{\varphi}_n &= -\tilde{\varphi}_n \\ \hat{\mathbb{P}}\varphi_n &= \varphi_n \end{aligned} \tag{6.101}$$

2 Suppose that at $t = 0$ the particle is in the state

$$\begin{aligned} \psi(x, 0) &= \sqrt{\frac{2}{45L}}\left[6 \sin\left(\frac{2\pi x}{L}\right) + 3 \cos\left(\frac{\pi x}{L}\right)\right] \\ &= \frac{1}{\sqrt{45}}(6\tilde{\varphi}_2 + 3\varphi_1) \end{aligned} \tag{6.102}$$

2. At $t > 0$,

$$\psi(x, t) = \sqrt{\frac{2}{45L}}\left[6 \sin\left(\frac{2\pi x}{L}\right)e^{-iE_2t/\hbar} + 3 \cos\left(\frac{\pi x}{L}\right)e^{-iE_1t/\hbar}\right] \tag{6.103}$$

6.16)

a) $\{\hat{\mathbb{P}}, \hat{p}\}\, g(x) = \hat{\mathbb{P}}\left(-i\hbar \frac{\partial}{\partial x}\, g(x)\right) + (-i\hbar)\frac{\partial}{\partial x}\left(\hat{\mathbb{P}}\, g(x)\right) =$

$-i\hbar\, \hat{\mathbb{P}}\, g'(x) + (-i\hbar)\frac{\partial}{\partial x}\left(g(-x)\right) = -i\hbar\, g'(-x) + (-i\hbar)(-1)\, g'(-x) =$

$-i\hbar\, g'(-x) + i\hbar\, g'(-x) = 0 \Rightarrow \{\hat{\mathbb{P}}, \hat{p}\} = 0$

(b) $[\hat{\mathbb{P}}, \hat{p}^2] = [\hat{\mathbb{P}}, \hat{p}]\,\hat{p} + \hat{p}\,[\hat{\mathbb{P}}, \hat{p}] =$

$\underline{\hat{\mathbb{P}}\hat{p}\hat{p}} - \hat{p}\hat{\mathbb{P}}\hat{p} + \underline{\hat{p}\hat{\mathbb{P}}\hat{p}} - \hat{p}\hat{p}\hat{\mathbb{P}} =$

$(\hat{\mathbb{P}}\hat{p} + \hat{p}\hat{\mathbb{P}})\,\hat{p} - \hat{p}(\hat{\mathbb{P}}\hat{p} + \hat{p}\hat{\mathbb{P}}) = \{\hat{\mathbb{P}}, \hat{p}\}\,\hat{p} - \hat{p}\,\{\hat{\mathbb{P}}, \hat{p}\} =$

$(0)\,\hat{p} - \hat{p}(0) = 0 \Rightarrow [\hat{\mathbb{P}}, \hat{p}]\, g(x) = 0 \ g(x)$

3 The expectation of $\mathbb{P}$ at $t = 0$ is

$$\langle \mathbb{P} \rangle = \langle \psi(x, 0) | \hat{\mathbb{P}} \psi(x, 0) \rangle \tag{6.104}$$

$$\hat{\mathbb{P}} \psi(x, 0) = \frac{1}{\sqrt{45}}(-6\tilde{\varphi}_2 + 3\varphi_1)$$

$$\langle \mathbb{P} \rangle = \frac{1}{45}\{-36\langle \tilde{\varphi}_2 | \tilde{\varphi}_2 \rangle + 9\langle \varphi_1 | \varphi_1 \rangle\} = -\frac{27}{45}$$

•2 Since $[\hat{\mathbb{P}}, H] = 0$, this is the value of $\langle \mathbb{P} \rangle$ for all time. In that the initial state (6.102) is
1 a superposition of the eigenstates of $\hat{\mathbb{P}}$, the squares of the coefficients of expansion give the probability that measurement finds the system in a state of even or odd parity.
2 Measurements on an ensemble of 4500 boxes all of whose particles are in the initial state (6.102) at the time $t = 0$ would find approximately 3600 of the particles in the odd state $\tilde{\varphi}_2(t)$ and approximately 900 of the particles in the even state $\varphi_1(t)$ at the subsequent time $t > 0$.

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PROBLEMS

6.16 (a) Show that $\hat{\mathbb{P}}$ *anticommutes* with the momentum operator $\hat{p}$. That is, show that

$$\{\hat{\mathbb{P}}, \hat{p}\} \equiv \hat{\mathbb{P}}\hat{p} + \hat{p}\hat{\mathbb{P}} = 0$$

(b) Use your answer to part (a) to show that $\hat{\mathbb{P}}$ commutes with the kinetic-energy operator $\hat{T} = \hat{p}^2/2m$.

6.17 A particle in one dimension is in the energy eigenstate

$$\varphi_{k_0} = A \cos(k_0 x)$$

Ideal measurement of energy finds the value

$$E = \frac{\hbar^2 {k_0}^2}{2m}$$

What is the state of the particle after measurement?

Answer

If we recall postulate II of quantum mechanics (Section 3.3), the system is left in the eigenstate of $\hat{H}$ corresponding to the eigenenergy above. Any state in the two-dimensional subspace of Hilbert space spanned by $\sin(k_0 x)$ and $\cos(k_0 x)$ [or, equivalently, $\exp(ik_0 x)$ and $\exp(-ik_0 x)$] gives the eigenenergy above. However, an *ideal measurement* perturbs the system least. In the state before measurement the probability distribution relating to momentum is 1/2 for $p = \pm\hbar k_0$. If we guess that the system is left in the state $\exp(ik_0 x)$ after measurement, the momentum distribution of the original state was disturbed. If we guess that the state of the measurement is $\sin(k_0 x)$, then measurement has not disturbed the momentum distribution; however, this measurement has disturbed the parity. In the original state the parity is $+1$ (with respect to the origin $x = 0$) while that of the hypothesized state after measurement is -1. This is still not the ideal measurement. We can find a measurement that perturbs the system even less. Consider that the particle is left in the state $\cos(k_0 x)$. The corresponding measurement did not perturb the momentum distribution or the parity of the original state. It is the ideal measurement.

6.18 (a) If $f(x)$ is any function, show that

$$f_+ = \frac{f(x) + f(-x)}{2} = \text{even function}$$

$$f_- = \frac{f(x) - f(-x)}{2} = \text{odd function}$$

(b) Show that

$$\hat{\mathbb{P}}_+ \equiv \frac{\hat{I} + \hat{\mathbb{P}}}{2}$$

is such that

$$\hat{\mathbb{P}}_+ f(x) = f_+(x)$$

The identity operator is $\hat{I}$.

(c) Show that

$$\hat{\mathbb{P}}_- \equiv \frac{\hat{I} - \hat{\mathbb{P}}}{2}$$

is such that

$$\hat{\mathbb{P}}_- f(x) = f_-(x)$$

The operator $\hat{\mathbb{P}}_+$ "projects" f onto f_+ while $\hat{\mathbb{P}}_-$ projects f onto f_-.

(d) Show that the *projection operators* $\hat{\mathbb{P}}_+$ and $\hat{\mathbb{P}}_-$ satisfy the following properties:

$$\hat{\mathbb{P}}_\pm{}^2 = \hat{\mathbb{P}}_\pm$$

$$[\hat{\mathbb{P}}_+, \hat{\mathbb{P}}_-] = 0$$

$$\hat{\mathbb{P}}_+ + \hat{\mathbb{P}}_- = \hat{I}$$

6.19 What is $\langle \mathbb{P} \rangle$ for a particle in a one-dimensional box with walls at $(-L/2, +L/2)$ in the initial state

$$\psi(x, 0) = \frac{1}{\sqrt{29}} (3\tilde{\varphi}_2 + 4\tilde{\varphi}_4 + 2\varphi_3)$$

6.20 For the same one-dimensional box as described in Problem 6.19, it is known that the particle is in a state with energy probabilities

$$P(E_1) = \tfrac{1}{3}, \quad P(E_2) = \tfrac{1}{3}, \quad P(E_3) = \tfrac{1}{3}$$

$$P(E_n) = 0, \quad (n \neq 1, 2, 3)$$

The parity of the state is measured ideally and -1 is found. If some time later E is measured, what value is found? What is the answer if the original measurement found the parity to be $+1$?

6.21 For a free particle moving in one dimension, divide the following set of operators into subsets of commuting operators.

$$\{\hat{\mathbb{P}}, \hat{x}, \hat{H}, \hat{p}\}$$

6.22 A free particle moving in one dimension is in the initial state $\psi(x, 0)$. Prove that $\langle p \rangle$ is constant in time by direct calculation (i.e., without recourse to the commutator theorem regarding constants of the motion).

Answer

With

$$\bar{b}(k, t) \equiv b(k)e^{i\omega t}$$

$$\frac{\hbar^2 k^2}{2m} = \hbar\omega$$

$$b(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(x, 0)e^{-ikx}\, dx$$

the expectation of p appears as

$$\langle p \rangle = \int_{-\infty}^{\infty} \hbar k |\bar{b}(k, t)|^2\, dk$$

which, given the structure of $\bar{b}(k, t)$ above, is time-independent. Alternatively, we may note that for a free-particle wave packet, $\hat{H} = \hat{p}^2/2m$, so that $d\langle p \rangle/dt = (1/i\hbar)\langle [H, p] \rangle = 0$.

6.23 In three dimensions, $\hat{\mathbb{P}}$ is defined as

$$\hat{\mathbb{P}}\psi(x, y, z) = \psi(-x, -y, -z)$$

(a) What does this definition become if ψ is measured in spherical coordinates: that is, $\psi = \psi(r, \theta, \phi)$?

(b) What does it become if ψ is measured in cylindrical coordinates: that is, $\psi = \psi(\rho, z, \phi)$?

(c) What are the parities of the following functions?

$$\psi_1 = A(x + y + z)e^{-(x^2 + y^2 + z^2)}$$

$$\psi_2 = Bre^{-r^2} \cos\theta$$

$$\psi_3 = C\frac{\sqrt{\rho^2 + z^2} \sin\phi}{z^5}$$

6.24 Discuss the consistency or inconsistency of the concept of the trajectory of a particle

$$\mathbf{r} = \mathbf{r}(t)$$

(whose mass is also known) in quantum mechanics.

Answer

The trajectory (through differentiation) implies the momentum, $\mathbf{p} = \mathbf{p}(t)$. Thus, at each instant, $\mathbf{r}$ and $\mathbf{p}$ are known, which is in violation of the uncertainty principle. On the other hand, for a wave packet one may construct the equation

$$\frac{d}{dt}\langle \mathbf{r} \rangle = \frac{1}{m}\langle \mathbf{p} \rangle$$

If $\langle \mathbf{p} \rangle$ is a known function of time, this equation may be integrated to obtain the trajectory, that is, $\langle \mathbf{r} \rangle$, as a function of time. The classical trajectory ensues when quantum fluctuations about the mean $\langle \mathbf{r} \rangle$ oscillate rapidly, thereby "averaging out." Equivalently, one may say that this limit is reached when the de Broglie wavelength is small compared to characteristic distances of the configuration.

6.25 Let a particle move in the potential

$$V = Ax^n$$

where A is constant and n is a finite integer. Show that Ehrenfest's equation (6.74) gives the classical relation

$$\frac{dp}{dt} = -Anx^{n-1}$$

only for $n = 2$ (the harmonic oscillator).

Answer

From (6.75) we obtain

$$\frac{d\langle p \rangle}{dt} = -An\langle x^{n-1} \rangle$$

To obtain the classical form we must equate $\langle x^{n-1} \rangle = \langle x \rangle^{n-1}$, which is only valid for $n = 2$.

6.26 (a) Consider that a particle is bound to the potential $V(x)$ and is initially in the state $\psi(x, 0)$. If eigenfunctions of the Hamiltonian $\hat{H} = \hat{p}^2/2m + V(x)$ are written $\varphi_n(x)$,

$$\hat{H}\varphi_n = E_n\varphi_n$$

obtain the state function $\psi(x, t)$ in terms of an integral over the propagator $K(x', x; t)$. That is, construct an explicit form for K as it appears in the integral

$$\psi(x, t) = \int \psi(x', 0)K(x', x; t)\, dx'$$

(b) Show that the propagator you have constructed satisfies the integral equation

$$K(x', x; t - t_0) = \int K(x', x''; t - t_1)K(x'', x; t_1 - t_0)\, dx''$$

Answer (*partial*)

(a) The formal solution to the time-dependent Schrödinger equation appears as (see Eq. 3.70)

$$\psi(x, t) = \exp\left(-\frac{it\hat{H}}{\hbar}\right)\psi(x, 0)$$

Expanding the initial state in eigenstates of $\hat{H}$ (see Eq. 5.6) gives

$$\psi(x, 0) = \sum_n b_n \varphi_n(x)$$

$$b_n = \int \psi(x', 0)\varphi_n^*(x')\, dx'$$

Substituting in the above gives

$$\begin{aligned}\psi(x, t) &= \sum_n b_n \exp\left(-\frac{iE_n t}{\hbar}\right)\varphi_n(x)\\ &= \int \psi(x', 0)\left[\sum_n \varphi_n^*(x')\varphi_n(x)e^{-iE_n t/\hbar}\right] dx'\\ &= \int \psi(x', 0)K(x', x; t)\, dx'\end{aligned}$$

which serves to identify the propagator

$$K(x', x; t) = \sum_n \varphi_n^*(x')\varphi_n(x)e^{-iE_n t/\hbar}$$

In Dirac notation this equation appears as

$$\hat{K}(x', x; t) = \sum_n |\varphi_n(x)\rangle e^{-iE_n t/\hbar}\langle\varphi_n(x')|$$

which allows the solution to be written:

$$|\psi(x, t)\rangle = \hat{K}\,|\,\psi(x, 0)\rangle$$

CHAPTER 7

ADDITIONAL ONE-DIMENSIONAL PROBLEMS. BOUND AND UNBOUND STATES

7.1 *General Properties of the One-Dimensional Schrödinger Equation*
7.2 *The Harmonic Oscillator*
7.3 *Eigenfunctions of the Harmonic Oscillator Hamiltonian*
7.4 *The Harmonic Oscillator in Momentum Space*
7.5 *Unbound States*
7.6 *One-Dimensional Barrier Problems*
7.7 *The Rectangular Barrier. Tunneling*
7.8 *The Ramsauer Effect*
7.9 *Kinetic Properties of a Wave Packet Scattered from a Potential Barrier*
7.10 *The WKB Approximation*

In this and the following chapters we examine some practical and fundamental problems in one dimension. Included are the very important examples of the harmonic oscillator and scattering configurations in one dimension. Creation and annihilation operators are introduced in algebraic construction of eigenenergies of the harmonic oscillator. The purely quantum mechanical effect of tunneling is encountered in a study of transmission through a barrier. The chapter concludes with a description of the WKB technique of solution appropriate in the near-classical domain. This method of approximation finds application in still more realistic configurations, such as cold emission from a metal surface and α decay from a radioactive nucleus.

7.1 GENERAL PROPERTIES OF THE ONE-DIMENSIONAL SCHRÖDINGER EQUATION

The time-independent Schrödinger equation for a particle of mass m moving in one dimension in a potential field $V(x)$ appears as

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\varphi(x) = E\varphi(x) \tag{7.1}$$

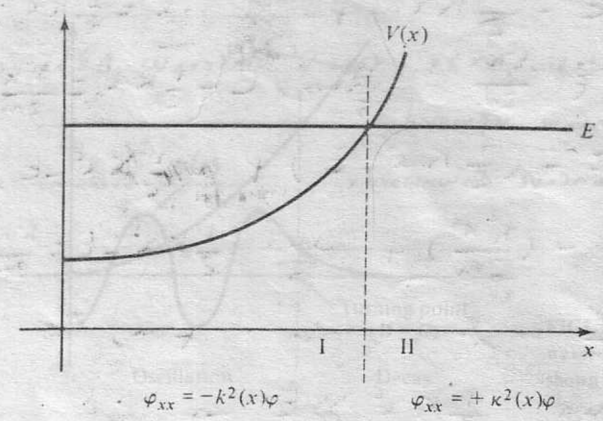
$V(x)$
E
I
II
x
$\varphi_{xx} = -k^2(x)\varphi$
$\varphi_{xx} = +\kappa^2(x)\varphi$

FIGURE 7.1 **Domains relevant to a particle of energy E moving in a one-dimensional potential field $V(x)$. I: $E > V$. Kinetic energy is positive. II: $E < V$. Kinetic energy is negative ("forbidden domain"). III: $E = V$. This is a *turning point* of the corresponding classical motion.**

1 With subscripts denoting differentiation, this equation may be rewritten

$$-\frac{2m}{\hbar^2}(E-V)\varphi = \varphi_{xx} = -k^2(x)\varphi \qquad \frac{1}{2m}\left(-i\hbar\frac{\partial}{\partial x}\right)^2\varphi = (E-V)\varphi \text{, but}$$

$$\hat{p}^2\varphi = (\hbar k)^2\varphi \Rightarrow$$

(7.2)
$$\frac{h^2k^2}{2m} = E - V \qquad \left(\frac{\hbar^2k^2}{2m}\right) = (E-V)$$

2 The partition of energy

(7.3)
$$E = T + V$$

permits us to identify $\hbar^2k^2/2m$ as the kinetic energy of the particle

(7.4)
$$T = \frac{h^2k^2}{2m}$$

$E > V \Rightarrow T > 0$
$E = V \Rightarrow T = 0$
$E < V \Rightarrow T < 0$

This identification is especially relevant if $E > V$. More generally, there are three distinct possibilities (Fig. 7.1). These are $E > V$, $E < V$, and $E = V$. In the first case 1 the kinetic energy is positive and the corresponding classical motion is permitted. Classical motion is forbidden in the second domain, where the kinetic energy is negative. The points where $E = V$ are the classical *turning points*. (Recall Section 1.4.)

2 In the domain where the kinetic energy is negative, the Schrödinger equation becomes

(7.5)
$$\varphi_{xx} = \kappa^2\varphi$$
$$\frac{\hbar^2\kappa^2}{2m} = V - E > 0$$

$$\text{kinetic energy} = -\frac{\hbar^2\kappa^2}{2m} = E - V < 0$$

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-2 Recall now that in analytic geometry, φ_{xx} is related to the *curvature* of φ (at
1 the point x). If $\varphi_{xx} > 0$, then φ is concave upward. If $\varphi_{xx} < 0$, then φ is concave down-
2 ward. When the kinetic energy is positive, the Schrödinger equation takes the form
· (7.2) and φ has the following properties: φ_{xx} is less than zero in the upper half-plane so φ is concave downward; φ_{xx} is greater than zero in the lower half-plane, so φ is concave upward. As shown in Fig. 7.2, these conditions permit *oscillating solutions.*

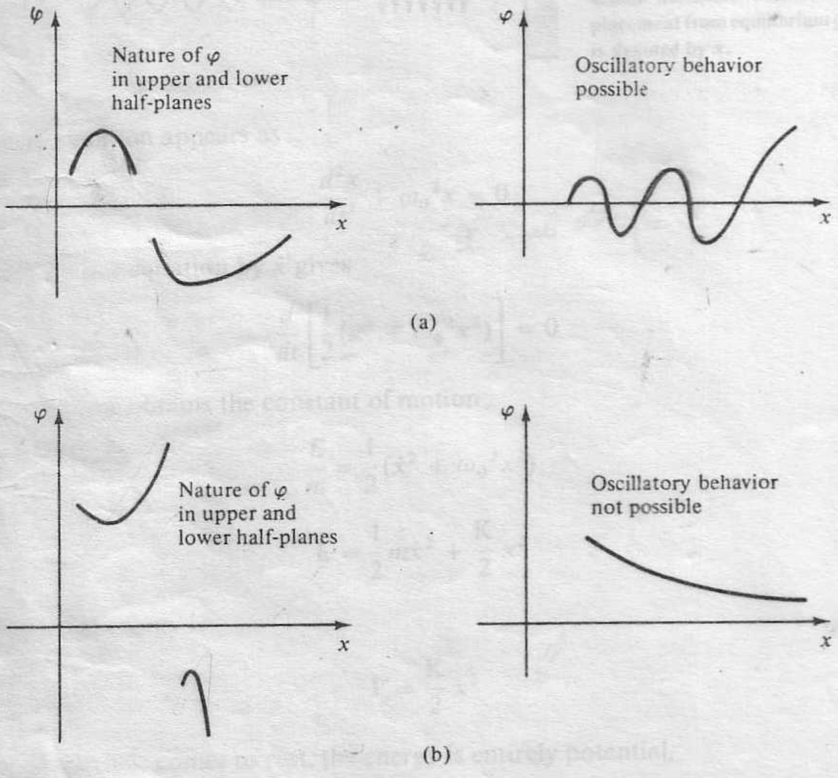


FIGURE 7.2 (a) Kinetic energy positive:

Use 1st

2 $\varphi_{xx} = -k^2\varphi \qquad k^2 > 0$

4 Concave downward. 1 $\varphi_{xx} < 0$ **for** $\varphi > 0$ **(upper half-plane)** 3

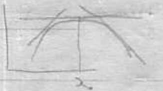
$\varphi_{xx} > 0$ **for** $\varphi < 0$ **(lower half-plane)**

(b) Kinetic energy negative:

$\varphi_{xx} = \kappa^2\varphi \qquad \kappa^2 > 0$

$\varphi_{xx} > 0$ **for** $\varphi > 0$ **(upper half-plane)**

$\varphi_{xx} < 0$ **for** $\varphi < 0$ **(lower half-plane)**



$$f' = \frac{df}{dx}\Big|_{x_0} = 0 \quad , \lim_{\Delta x \to 0} \frac{f'(x+\Delta x) - f'(x)}{\Delta x} = \frac{d^2 f}{dx^2} \quad \begin{array}{l} (1) < 0 \\ (2) > 0 \end{array}$$

(1) f' decreases , $\Delta x > 0$; (2) f' increases , $\Delta x > 0$

(1) $\frac{d^2 f}{dx^2} > 0$ minima i.e Concave upward

(2) $\frac{d^2 f}{dx^2} < 0$ maxima i.e Concave downward.

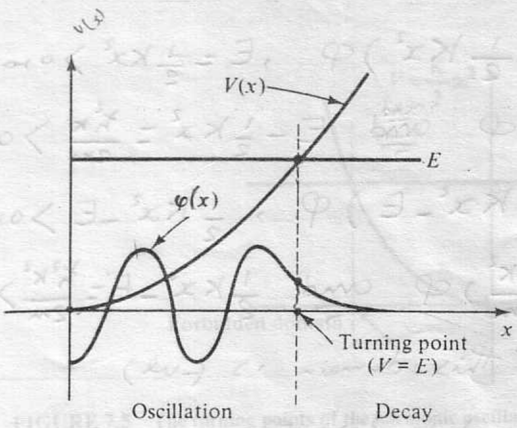


FIGURE 7.3 Characteristic behavior of wavefunction corresponding to the configuration shown in Fig. 7.1.

3 When the kinetic energy is negative, the Schrödinger equation takes the form (7.5) and the following properties pertain: φ_{xx} is greater than zero in the upper half-plane so φ is concave upward; φ_{xx} is less than zero in the lower half-plane and φ is
3 concave downward. Again referring to Fig. 7.2, these conditions are seen to lead to
ازدياد - نقص
growing or decaying solutions (as opposed to oscillating solutions). At a turning
4 point, $\varphi_{xx} = 0$ and φ has a constant slope.

For the potential shown in Fig. 7.1, one might then expect an eigenfunction of the Hamiltonian to behave as depicted in Fig. 7.3.

PROBLEMS

7.1 (a) Let a particle of mass m move in a one-dimensional potential field with energy E as sketched in Fig. 1.18. Write down the form of the time-independent Schrödinger equation (i.e., Eq. 7.2 or Eq. 7.5) for the four domains that lie in the interval $0 \leq x \leq D$. In each case identify the wavenumber k or κ.

(b) **Given** $\varphi(0) = \varphi_0 > 0$, make a rough sketch of $\varphi(x)$ in the interval $0 \leq x \leq F$.

7.2 THE HARMONIC OSCILLATOR

The configuration of a harmonic oscillator is depicted in Fig. 7.4. The classical equation of motion of a particle of mass m is given by Hooke's law,

$$m\frac{d^2x}{dt^2} = -\mathrm{K}x \tag{7.6}$$

The spring constant is K. In terms of the natural frequency ω_0,

$$\omega_0{}^2 = \frac{\mathrm{K}}{m} \tag{7.7}$$

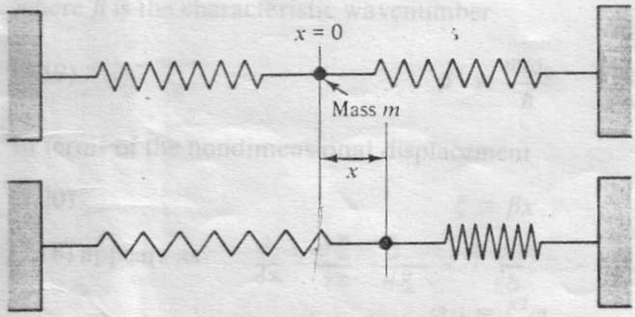


FIGURE 7.4 The one-dimensional harmonic oscillator. Displacement from equilibrium ($x = 0$) is denoted by x.

the above equation appears as

(7.8) $$\frac{d^2x}{dt^2} + {\omega_0}^2 x = 0$$

$\dot{x}\ddot{x} + \omega_0^2 \dot{x}x = 0$

1 Multiplying this equation by $\dot{x}$ gives

(7.9) $$\frac{d}{dt}\left[\frac{1}{2}(\dot{x}^2 + {\omega_0}^2 x^2)\right] = 0$$

Integrating, one obtains the constant of motion

(7.10) $$\frac{E}{m} = \frac{1}{2}(\dot{x}^2 + {\omega_0}^2 x^2)$$
$$E = \frac{1}{2}m\dot{x}^2 + \frac{K}{2}x^2$$

2 The potential energy is

(7.11) $$V = \frac{K}{2}x^2$$

2 When the particle comes to rest, the energy is entirely potential.

(7.12) $$E = \frac{K}{2}{x_0}^2$$ at x = constant = x_0

3 Such points (x_0) are turning points. For $x^2 > {x_0}^2$, the kinetic energy T is negative, so that classically this is a forbidden domain.

(7.13) $$T = E - V = \frac{K}{2}({x_0}^2 - x^2)$$
$$T < 0 \qquad (\text{for } x^2 > {x_0}^2)$$

In classical

See Fig. 7.5.

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\varphi + \frac{1}{2}Kx^2\varphi = E\varphi \quad \Rightarrow$$

1 When $-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\varphi = (E - \frac{1}{2}Kx^2)\varphi$, $E - \frac{1}{2}Kx^2 > 0 \rightarrow$

$= (\frac{\hbar^2 k^2}{2m})\varphi$ and $\Rightarrow$ $E - \frac{1}{2}Kx^2 = \frac{\hbar^2 k^2}{2m} > 0$

2 When $-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\varphi = -(\frac{1}{2}Kx^2 - E)\varphi$, $\frac{1}{2}Kx^2 - E > 0 \rightarrow$

$\rightarrow$ $= \boxed{-}(\frac{\hbar^2 k^2}{2m})\varphi$ and $\Rightarrow$ $\frac{1}{2}Kx^2 - E = \frac{\hbar^2 k^2}{2m} > 0$

the $\boxed{-}$ is because $\frac{\hat{p}^2}{2m}$ in this domain is (−ve)

3 In the asymptotic domain $\frac{1}{2}Kx^2 \gg E \rightarrow$

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\varphi - \frac{1}{2}Kx^2\varphi = \frac{\hbar^2 k^2}{2m} \rightarrow$$

$$\varphi_{xx} - \frac{mK}{\hbar^2}x^2\varphi - k^2\varphi = \beta^4 x^2\varphi$$

$$\frac{m\,\boxed{m}\,K}{\hbar^2\,\boxed{m}} = \frac{m^2\omega_0^2}{\hbar^2} = (\frac{m\omega_0}{\hbar})^2 = \beta^4 \Rightarrow \beta^2 = \frac{m\omega_0}{\hbar}$$

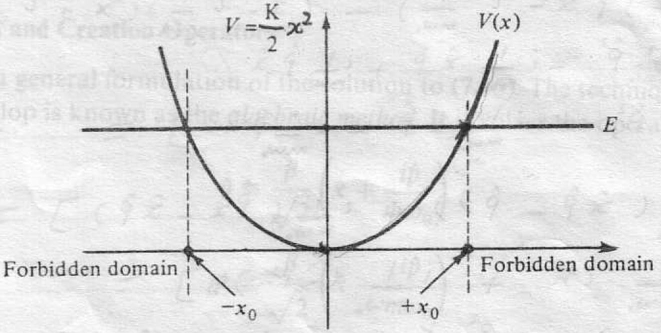


FIGURE 7.5 The turning points of the harmonic oscillator are at $x = \pm x_0$, where

$$\frac{Kx_0^2}{2} = E$$

In Q.M

1 With these properties of the classical motion established, we turn next to the quantum mechanical formulation of the harmonic oscillator problem. The Hamiltonian for a particle of mass m in the potential (7.11) is

$$H = \frac{p^2}{2m} + \frac{K}{2}x^2 \qquad (7.14)$$

4

The corresponding Schrödinger equation appears as

$$-\frac{\hbar^2}{2m}\frac{\partial^2\varphi}{\partial x^2} + \frac{K}{2}x^2\varphi = E\varphi \qquad (7.15)$$

1 In the classically accessible domain, $E > Kx^2/2$, and this equation may be written

[illegible]

$$\varphi_{xx} = -k^2\varphi$$
$$\frac{\hbar^2 k^2(x)}{2m} = E - \frac{K}{2}x^2 > 0 \qquad (7.16)$$

The wavefunction φ is oscillatory in this domain.

2 In the classically forbidden domain where $x^2 > x_0^2$, $E < Kx^2/2$ and the Schrödinger equation becomes

$$\varphi_{xx} = \kappa^2\varphi$$
$$\frac{\hbar^2\kappa^2}{2m} = \frac{K}{2}x^2 - E > 0 \qquad (7.17)$$

$\frac{K}{2}x^2 \gg E \mapsto \frac{\hbar^2\kappa^2}{2m} = \frac{K}{2}x^2 \Rightarrow$
$\varphi_{xx} = \kappa^2\varphi = \frac{mK}{\hbar^2}x^2\varphi$
$(mK/\hbar^2) = \beta^4$

So the wavefunction is nonoscillatory in this domain. In the asymptotic domain $Kx^2/2 \gg E$, the Schrödinger equation becomes

$$\varphi_{xx} = \frac{mK}{\hbar^2}x^2\varphi \equiv \beta^4 x^2\varphi \qquad (7.18)$$

$\frac{K}{m} = \omega_0^2 \Rightarrow \frac{\boxed{m}K}{m\hbar^2} = \frac{\boxed{m}\omega_0^2}{\hbar^2} = \frac{\beta^4}{m}$

where β is the characteristic wavenumber

$$\beta^2 \equiv \frac{m\omega_0}{\hbar} \tag{7.19}$$

$$\frac{\cancel{(\text{mass})}\cdot(1/\text{sec.})}{\cancel{(\text{mass})}[(\text{distance})/\cancel{\text{sec}^2}]\ \text{distance}\cdot\cancel{\text{sec.}}}$$

In terms of the nondimensional displacement

$$\xi \equiv \beta x \tag{7.20}$$

$$\beta^4 x^2 = \beta^2(\beta^2 x^2) = \beta^2 \xi^2$$

$$\frac{d^2}{dx^2}\varphi = \beta^2 \xi^2 \varphi .$$

(7.18) appears as

$$\frac{d}{dx} = \frac{d\xi}{dx}\frac{d}{d\xi} = \beta\frac{d}{d\xi} \Rightarrow \frac{d^2}{dx^2} = \left(\frac{d}{dx}\right)^2 = \beta^2\frac{d^2}{d\xi^2}$$

$$\varphi_{\xi\xi} = \xi^2\varphi$$

In the domain under consideration, $\xi \gg 1$ and the solution to the latter equation appears as

$$\varphi \sim A \exp\left(\pm\frac{\xi^2}{2}\right) = A \exp\left[\pm\frac{(\beta x)^2}{2}\right]$$

The growing solution (+) violates the normalization condition

$$\int_{-\infty}^{\infty} \varphi^*\varphi\, dx < \infty \tag{7.21}$$

and one is left with the exponentially decaying wavefunction

$$\varphi \sim A \exp\left(-\frac{\xi^2}{2}\right) = A \exp\left[-\frac{(\beta x)^2}{2}\right] \tag{7.22}$$

The character of the wavefunction changes from oscillatory for $x^2 < x_0{}^2$ to decaying for $x^2 > x_0{}^2$, so the turning points $x = \pm x_0$ are also physically relevant in quantum mechanics. These properties are depicted in Fig. 7.6.

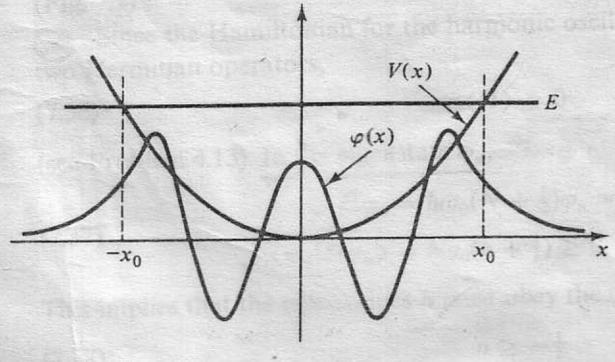


FIGURE 7.6 Typical behavior of energy eigenfunction for the simple harmonic oscillator.

$$\hat{x}\hat{p} - \hat{p}\hat{x} = i\hbar \quad , \; [\hat{a}, \hat{a}^{+}] = a\hat{a}^{+} - a^{+}a =$$

$$\frac{\beta^2}{2}\left[(\hat{x} + i\frac{\hat{p}}{m\omega_0})(\hat{x} - i\frac{\hat{p}}{m\omega_0}) - (\hat{x} - i\frac{\hat{p}}{m\omega_0})(\hat{x} + i\frac{\hat{p}}{m\omega_0})\right] =$$

$$\frac{\beta^2}{2}\left[\cancel{\hat{x}^2} + \cancel{(\frac{1}{m\omega_0})^2\hat{p}^2} - i\frac{1}{m\omega_0}\hat{x}\hat{p} + i\frac{1}{m\omega_0}\hat{p}\hat{x}\right.$$

$$\left. -1(\cancel{\hat{x}^2} + \cancel{(\frac{1}{m\omega_0})^2\hat{p}^2} + i\frac{1}{m\omega_0}\hat{x}\hat{p} - i\frac{1}{m\omega_0}\hat{p}\hat{x}\right] =$$

$$\frac{\beta^2}{2}\left[-i\frac{1}{m\omega_0}(\hat{x}\hat{p} - \hat{p}\hat{x}) + i\frac{1}{m\omega_0}(\hat{p}\hat{x} - \hat{x}\hat{p})\right] =$$

$$\frac{\beta^2}{2}\left[-i\frac{1}{m\omega_0}(i\hbar + i\frac{1}{m\omega_0}(-i\hbar)\right] =$$

$$\frac{\beta^2}{\cancel{2}}(\cancel{2}\frac{\hbar}{m\omega_0}) = \beta^2\frac{\hbar}{m\omega_0} = 1 = [\hat{a}, \hat{a}^{+}]$$

$$* \quad \beta^4 = \frac{\cancel{mK}}{\hbar^2} = \frac{m\,\textcircled{m}}{\hbar^2}\frac{K}{\textcircled{m}} = \frac{m^2}{\hbar^2}\omega_0^2 = (\frac{m\omega_0}{\hbar})^2 \Rightarrow$$

$$\beta^2 = \frac{m\omega_0}{\hbar} \Rightarrow \beta^2\frac{1}{\beta^2} = 1 \; ; \quad \frac{K}{m} = \omega_0^2 \Rightarrow K = m\omega_0^2$$

$$* \quad \hat{x}^2 = (\frac{1}{\sqrt{2}\beta})^2(\hat{a} + \hat{a}^{+})(\hat{a} + \hat{a}^{+}) = \frac{1}{2\beta^2}\left[\hat{a}^2 + \hat{a}^{+2} + (\hat{a}^{+}\hat{a} + \hat{a}\hat{a}^{+})\right]$$

$$\hat{p}^2 = (\frac{m\omega_0}{i\sqrt{2}\beta})^2(\hat{a} - \hat{a}^{+})(\hat{a} - \hat{a}^{+}) = -\frac{1}{2}(\frac{m\omega_0}{\beta})^2\left[\hat{a}^2 + \hat{a}^{+2} - (\hat{a}\hat{a}^{+} + \hat{a}^{+}\hat{a})\right]$$

$$\Rightarrow \frac{1}{2m}\hat{p}^2 = -(\frac{1}{2})^2\frac{m^{\textcircled{2}}\omega_0^2}{\textcircled{m}\,\beta^2}[\;[\;]\;] = -\frac{1}{4}\frac{m\omega_0}{\hbar}\frac{\hbar\omega_0}{\beta^2} = -\frac{1}{4}\hbar\omega_0[\boxed{1}]$$

$$\frac{K}{2}\hat{x}^2 = \frac{1}{2}\textcircled{m}\,\omega_0^{\textcircled{2}}(\frac{1}{2}\frac{\hbar}{\textcircled{m\omega_0}}) = \frac{1}{4}\hbar\omega_0[\boxed{2}] =$$

$$\frac{1}{2m}\hat{p}^2 + \frac{1}{2}K\hat{x}^2 = \frac{1}{4}\hbar\omega_0(\boxed{2} - \boxed{1}) = \frac{1}{2}\frac{1}{\cancel{2}}\hbar\omega_0(\cancel{2}(\hat{a}\hat{a}^{+} + \hat{a}^{+}\hat{a})) =$$

$$\frac{1}{2}\hbar\omega_0(1 + \hat{a}^{+}\hat{a} + \hat{a}^{+}\hat{a}) = \frac{1}{2}\hbar\omega_0(1 + 2\hat{a}^{+}\hat{a}) = \frac{\cancel{2}}{\cancel{2}}\hbar\omega_0(\hat{a}^{+}\hat{a} + \frac{1}{2})$$

Annihilation and Creation Operators

We turn to a general formulation of the solution to (7.15). The technique of solution we will develop is known as the *algebraic method.* It involves the operators

$$\hat{a} \equiv \frac{\beta}{\sqrt{2}}\left(\hat{x} + \frac{i\hat{p}}{m\omega_0}\right) \tag{7.23}$$

$$\hat{a}^\dagger = \frac{\beta}{\sqrt{2}}\left(\hat{x} - \frac{i\hat{p}}{m\omega_0}\right)$$

Inasmuch as $\hat{a} \neq \hat{a}^\dagger$, $\hat{a}$ is non-Hermitian. The properties that these operators have are determined through the fundamental commutator relation

$$[\hat{x}, \hat{p}] = i\hbar \tag{7.24}$$

For instance, it is readily shown that (see Problem 7.5)

$$[\hat{a}, \hat{a}^\dagger] = 1 \tag{7.25}$$

$$\hat{a}\hat{a}^\dagger = 1 + \hat{a}^\dagger\hat{a}$$

With the aid of the inverse of (7.23),

$$\hat{x} = \frac{\hat{a} + \hat{a}^\dagger}{\sqrt{2}\beta}, \qquad \hat{p} = \frac{m\omega_0}{i}\frac{\hat{a} - \hat{a}^\dagger}{\sqrt{2}\beta} \tag{7.26}$$

the Hamiltonian for the harmonic oscillator becomes

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{K\hat{x}^2}{2} = \hbar\omega_0(\hat{a}^\dagger\hat{a} + \tfrac{1}{2}) \tag{7.27}$$

In this manner we see that the problem of finding the eigenvalues of $\hat{H}$ has been transformed to that of finding the eigenvalues of the operator

$$\hat{N} \equiv \hat{a}^\dagger\hat{a} \tag{7.28}$$

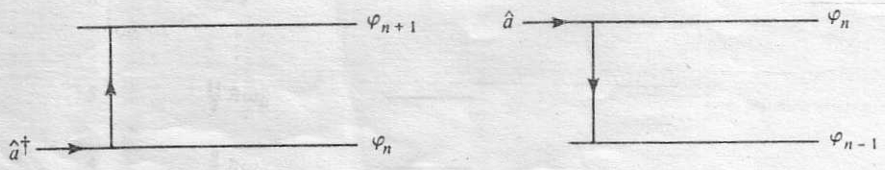
Let φ_n be the eigenfunction of $\hat{N}$ corresponding to the eigenvalue n, so that

$$\hat{N}\varphi_n = n\varphi_n \tag{7.29}$$

(We do not assume that n is an integer at this point. This property is established later.) Consider the effect of operating on $\hat{a}\varphi_n$ with $\hat{N}$.

$$\hat{N}\hat{a}\varphi_n = \hat{a}^\dagger\hat{a}\hat{a}\varphi_n = (\hat{a}\hat{a}^\dagger - 1)\hat{a}\varphi_n = \hat{a}(\hat{a}^\dagger\hat{a} - 1)\varphi_n \tag{7.30}$$

$$\hat{N}\hat{a}\varphi_n = \hat{a}(\hat{N} - 1)\varphi_n = \hat{a}(n - 1)\varphi_n = (n - 1)\hat{a}\varphi_n$$



(a) (b)

FIGURE 7.7 Schematic representation of the raising and lowering operators $\hat{a}^\dagger$ and $\hat{a}$.

2· It follows that $\hat{a}\varphi_n$ is the eigenfunction of $\hat{N}$ which corresponds to the eigenvalue $n-1$. That is (apart from normalization factors),

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(7.31) $$\hat{a}\varphi_n = \varphi_{n-1}$$

Similarly,

(7.32) $$\hat{a}\varphi_{n-1} = \varphi_{n-2}$$

فناء

and so forth. Because of this property, $\hat{a}$ is called an *annihilation* or *stepdown* or *demotion* operator.

تخفيض

3 In similar manner, if we consider the operation $\hat{N}\hat{a}^\dagger\varphi_n$, there results

(7.33) $$\hat{N}\hat{a}^\dagger\varphi_n = (n+1)\hat{a}^\dagger\varphi_n$$

3· This equation implies that $\hat{a}^\dagger\varphi_n$ is the eigenfunction of $\hat{N}$ corresponding to the eigenvalue $n+1$.

(7.34) $$\hat{a}^\dagger\varphi_n = \varphi_{n+1}$$

Similarly,

(7.35) $$\hat{a}^\dagger\varphi_{n+1} = \varphi_{n+2}$$

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and so forth. The operator $\hat{a}^\dagger$ is called a *creation* or *stepup* or *promotion* operator (Fig. 7.7).

·2 (*) Since the Hamiltonian for the harmonic oscillator is the sum of the squares of two Hermitian operators,

(7.36) $$\langle H\rangle \geq 0$$

1 (see Problem 4.13). In the eigenstate φ_n,

(7.37) $$\because\ \hat{H}\varphi_n = \hbar\omega_0(\hat{N}+\tfrac{1}{2})\varphi_n = \hbar\omega_0(n+\tfrac{1}{2})\varphi_n$$
$$\therefore\ \langle\varphi_n|\hat{H}\varphi_n\rangle = \hbar\omega_0(n+\tfrac{1}{2}) \geq 0$$

2 This implies that the eigenvalues n must obey the condition

(7.38) $$n \geq -\tfrac{1}{2}$$

$$\hat{N}\hat{a}^{\dagger}\varphi_n = \hat{a}^{\dagger}\hat{a}\hat{a}^{\dagger}\varphi_n = \hat{a}^{\dagger}(1+\hat{a}^{\dagger}\hat{a})\varphi_n = \hat{a}^{\dagger}(1+n)\varphi_n = (n+1)\hat{a}^{\dagger}\varphi_n$$

.3 That is, all eigenstates of $\hat{H}$, or equivalently $\hat{N}$, corresponding to eigenvalues $n < -\frac{1}{2}$ must vanish identically. For the harmonic oscillator such states do not exist. This condition is guaranteed if we set

معنوي يكون

$$\hat{a}\varphi_0 = 0 \tag{7.39}$$

With (7.31) we obtain

$$\begin{aligned} \hat{a}\varphi_0 &= \varphi_{-1} = 0 \\ \hat{a}(\varphi_{-1}) &= \varphi_{-2} = 0 \end{aligned} \tag{7.40}$$

[illegible]

† As will be shown, (7.39) has a nontrivial (i.e., other than zero) solution for φ_0. Further-
1 more,

$$\hat{N}\varphi_0 = \hat{a}^\dagger\hat{a}\varphi_0 = 0 = 0\varphi_0 \tag{7.41}$$

* and we may conclude that the eigenvalue of $\hat{N}$ corresponding to the eigenfunction
2 φ_0 is zero. It follows that

$$\begin{aligned} \hat{N}\hat{a}^\dagger\varphi_0 &= \hat{a}^\dagger\underline{\hat{a}\hat{a}^\dagger}\varphi_0 = \hat{a}^\dagger(\hat{a}^\dagger\hat{a} + 1)\varphi_0 = \hat{a}^\dagger\varphi_0 \\ \therefore \hat{N}\varphi_1 &= \underline{\hat{N}\hat{a}^\dagger\varphi_0 = 1\hat{a}^\dagger\varphi_0 = \varphi_1} \end{aligned} \tag{7.42}$$

.4 The eigenvalue of $\hat{N}$ corresponding to φ_1 is the integer 1. This construction (same as in Eq. 7.34 et seq.) allows one to conclude that the index n, which labels the eigenfunction φ_n, is indeed an integer.

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→ Repeating (7.37),

$$\hat{H}\varphi_n = \hbar\omega_0(n + \tfrac{1}{2})\varphi_n \tag{7.43}$$

· one finds that the energy eigenvalues of the simple harmonic oscillator are

$$E_n = \hbar\omega_0(n + \tfrac{1}{2}) \qquad (n = 0, 1, 2, \ldots) \tag{7.44}$$

† The energy levels are equally spaced by the interval $\hbar\omega_0$ (Fig. 7.8). If a molecule, for
1 example HCl, which resembles a dumbbell, has vibrational modes of excitation (the arm of the dumbbell acts as a spring), the Bohr frequencies emitted by the molecule fall in the scheme – تردد - مخطط - [illegible]

$$\begin{aligned} h\nu = E_{n'} - E_n &= \hbar\omega_0(n' + \tfrac{1}{2}) - \hbar\omega_0(n + \tfrac{1}{2}) \\ &= \hbar\omega_0(n' - n) = \hbar\omega_0 s \\ \boxed{\nu = s\nu_0,} &\qquad \omega_0 \equiv 2\pi\nu_0 \end{aligned} \tag{7.45}$$

→ S: integer value

2 In the latter sequence of equations, n and n' are integers, so their difference, s, is also
3 an integer. It follows that the frequencies emitted by a vibrational diatomic molecule are integral multiples of the natural frequency of the molecule, ν_0 (Fig. 7.9).

$E = \frac{1}{2} w$

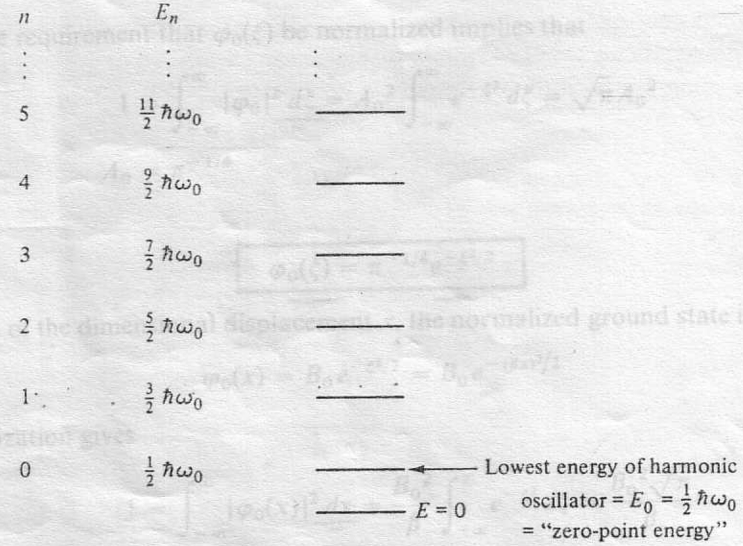
n
E_n
5
$\frac{11}{2}\hbar\omega_0$
4
$\frac{9}{2}\hbar\omega_0$
3
$\frac{7}{2}\hbar\omega_0$
2
$\frac{5}{2}\hbar\omega_0$
1
$\frac{3}{2}\hbar\omega_0$
0
$\frac{1}{2}\hbar\omega_0$
Lowest energy of harmonic oscillator = $E_0 = \frac{1}{2}\hbar\omega_0$ = "zero-point energy"
$E = 0$

FIGURE 7.8 The energy levels of the simple harmonic oscillator are equally spaced.

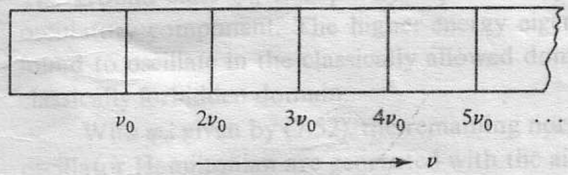

FIGURE 7.9 Spectrum of a vibrational diatomic molecule.

PROBLEMS

7.2 A harmonic oscillator consists of a mass of 1 g on a spring. Its frequency is 1 Hz and the mass passes through the equilibrium position with a velocity of 10 cm/s. What is the order of magnitude of the quantum number associated with the energy of the system?

7.3 The spacing between vibrational levels of the CO molecule is 2170 cm^{-1}. Taking the mass of C to be 12 amu and O to be 16 amu, compute the effective spring constant K, which is a measure of the bond stiffness between the atoms of the molecule. [*Hint:* The mass that enters is the reduced mass, $mM/m + M$. The spacing between lines is given in terms of wavenumber $k = 2\pi/\lambda$, where $\omega = ck$ (c = the speed of light), so that $\Delta\omega = c\,\Delta k$.]

قيد

7.4 The derivation in the text of the eigenvalues of $\hat{N}$ is based on the constraint that there are no states corresponding to the eigenvalues $n < -\frac{1}{2}$. This constraint was guaranteed by setting $\hat{a}\varphi_0 = 0$. It would appear that it can also be guaranteed by setting $\hat{a}\varphi_{1/2} = 0$, for in this case

$$\hat{a}\varphi_{1/2} = \varphi_{-1/2} = 0$$

(7.3) $\kappa = \frac{2\pi}{\lambda} = 2170\ \mathrm{cm}^{-1}$, $m_C = 12$ amu , $m_O = 16$ amu , $K = m\omega^2$?

$m = \frac{m_O m_C}{m_C + m_O} = \frac{12 \times \cancel{16}^{4}}{\cancel{28}_{7}} = \frac{48}{7}$, $C = (2\pi\nu)\frac{\lambda}{2\pi} = \omega\frac{1}{\kappa}$

$\kappa c = \omega \Rightarrow K = m(\kappa c)^2 = \frac{48}{7}(2170 \times 3 \times 10^8)^2 = K$

1 $\xi = \beta x = (\frac{m\omega_0}{\hbar})^{1/2} x \to \frac{\partial\xi}{\partial x} = \beta$; $\frac{\partial}{\partial x} = \frac{\partial\xi}{\partial x}\frac{\partial}{\partial\xi} = \beta\frac{\partial}{\partial\xi}$

$\hat{a} = \frac{\beta}{\sqrt{2}}(x + i\frac{\hat{P}}{m\omega_0}) = \frac{\beta}{\sqrt{2}}(x + \frac{i(-i)\hbar}{m\omega_0}\frac{\partial}{\partial x}) =$, $(\frac{\hbar}{m\omega_0}) = \frac{1}{\beta^2}$

$\frac{\beta}{\sqrt{2}}(x + \frac{1}{\beta}\frac{\partial}{\partial x}) = \frac{\beta}{\sqrt{2}}(\frac{\xi}{\beta} + \frac{1}{\beta^2}\beta\frac{\partial}{\partial\xi}) = \frac{1}{\sqrt{2}}(\xi + \frac{\partial}{\partial x})$

2 $\hat{H} = \hbar\omega_0(\hat{a}^{+}\hat{a} + \frac{1}{2})$, $\hat{a}^{+}\hat{a} = \frac{1}{2}(\xi - \frac{\partial}{\partial\xi})(\xi + \frac{\partial}{\partial\xi})$

$= \frac{1}{2}\left(\xi^2 + \underline{\xi\frac{\partial}{\partial\xi} - \frac{\partial}{\partial\xi}\xi} - (\frac{\partial}{\partial\xi})^2\right)$,

$\frac{\partial}{\partial\xi}(\xi\varphi) = \xi\frac{\partial}{\partial\xi}\varphi + \varphi \to$

$\xi\frac{\partial}{\partial\xi}\varphi - \frac{\partial}{\partial\xi}(\xi\varphi) = -\varphi \to \hat{H} = \hbar\omega_0(\hat{a}^{+}\hat{a} + \frac{1}{2})$

$\hat{H} = \hbar\omega_0[\frac{1}{2}(\xi^2 - (\frac{\partial}{\partial\xi})^2 - 1) + \frac{1}{2}] =$

$\hat{H}\varphi = \frac{\hbar\omega_0}{2}(\xi^2\varphi - \varphi_{\xi\xi}) = E\varphi \to$

$\varphi_{\xi\xi} + [(\frac{2E}{\hbar\omega_0}) - \xi^2]\varphi = 0$

$\hbar\omega\hat{\sigma} = \hbar\omega_0\left(n+\frac{1}{2}\right)$

Show that $\varphi_{1/2}$ as defined is an eigenfunction of $\hat{N}$ with the eigenvalue zero, hence $\varphi_{1/2}$ is more properly termed φ_0.

7.5 Using the fundamental commutator relation

$$[\hat{x}, \hat{p}] = i\hbar$$

show that

$$[\hat{a}, \hat{a}^\dagger] = 1$$

7.3 EIGENFUNCTIONS OF THE HARMONIC OSCILLATOR HAMILTONIAN

When written in terms of the nondimensional displacement ξ (7.20),

$$\xi^2 \equiv \frac{m\omega_0}{\hbar}x^2 \equiv \beta^2 x^2 \tag{7.46}$$

the operators $\hat{a}$ and $\hat{a}^\dagger$ become

$$\begin{aligned} \hat{a} &= \frac{\beta}{\sqrt{2}}\left(\hat{x} + \frac{i\hat{p}}{m\omega_0}\right) = \frac{\beta}{\sqrt{2}}\left(x + \frac{\hbar}{m\omega_0}\frac{\partial}{\partial x}\right) = \frac{1}{\sqrt{2}}\left(\xi + \frac{\partial}{\partial \xi}\right) \\ \hat{a}^\dagger &= \frac{\beta}{\sqrt{2}}\left(\hat{x} - \frac{i\hat{p}}{m\omega_0}\right) = \frac{\beta}{\sqrt{2}}\left(x - \frac{\hbar}{m\omega_0}\frac{\partial}{\partial x}\right) = \frac{1}{\sqrt{2}}\left(\xi - \frac{\partial}{\partial \xi}\right) \end{aligned} \tag{7.47}$$

1 The time-independent Schrödinger equation becomes

$$\left(2\hat{a}^\dagger\hat{a} + 1 - \frac{2E}{\hbar\omega_0}\right)\varphi = \varphi_{\xi\xi} + \left(\frac{2E}{\hbar\omega_0} - \xi^2\right)\varphi = 0 \tag{7.48}$$

2 The ground-state wavefunction φ_0 of the simple harmonic oscillator Hamiltonian obeys (7.39)

$$\hat{a}\varphi_0 = 0$$

or, equivalently,

$$\left(\xi + \frac{\partial}{\partial \xi}\right)\varphi_0 = 0 \tag{7.49}$$

This has the solution

$$\varphi_0 = A_0 e^{-\xi^2/2} \tag{7.50}$$

5

The requirement that $\varphi_0(\xi)$ be normalized implies that

$$1 = \int_{-\infty}^{\infty} |\varphi_0|^2 \, d\xi = A_0{}^2 \int_{-\infty}^{\infty} e^{-\xi^2} \, d\xi = \sqrt{\pi} A_0{}^2 \tag{7.51}$$

$$A_0 = \pi^{-1/4}$$

so

$$\boxed{\varphi_0(\xi) = \pi^{-1/4} e^{-\xi^2/2}} \tag{7.52}$$

In terms of the dimensional displacement x, the normalized ground state is

$$\varphi_0(x) = B_0 e^{-\xi^2/2} = B_0 e^{-(\beta x)^2/2} \tag{7.53}$$

Normalization gives

$$1 = \int_{-\infty}^{\infty} |\varphi_0(x)|^2 \, dx = \frac{B_0{}^2}{\beta} \int_{-\infty}^{\infty} e^{-\xi^2} \, d\xi = \frac{B_0{}^2 \sqrt{\pi}}{\beta}$$

$$\varphi_0(x) = \left(\frac{\beta^2}{\pi}\right)^{1/4} e^{-(\beta x)^2/2} \tag{7.54}$$

The ground state φ_0 is a purely exponentially decaying wavefunction. It has no oscillatory component. The higher-energy eigenstates, on the other hand, will be found to oscillate in the classically allowed domain and decay exponentially in the classically forbidden domain.

With φ_0 given by (7.52), the remaining normalized eigenstates of the harmonic oscillator Hamiltonian are generated with the aid of the creation operator $\hat{a}^\dagger$, in the following manner:

$$\varphi_1 = \hat{a}^\dagger \varphi_0$$

$$\varphi_2 = \frac{1}{\sqrt{2}} \hat{a}^\dagger \varphi_1 = \frac{1}{\sqrt{2}} (\hat{a}^\dagger)^2 \varphi_0 \tag{7.55}$$

$$\varphi_n = \frac{1}{\sqrt{n!}} (\hat{a}^\dagger)^n \varphi_0$$

?

With $\hat{a}^\dagger$ written in terms of ξ, as in (7.47), the equation for φ_1 above becomes

$$\varphi_1 = A_1 \left(\xi - \frac{\partial}{\partial \xi}\right) e^{-\xi^2/2}$$

$$\varphi_1 = A_1 2\xi e^{-\xi^2/2} \tag{7.56}$$

$$A_1 = (2\sqrt{\pi})^{-1/2}$$

We already know that φ_0 is normalized, dose this necessarily imply that $\varphi_n = (\hat{a}^{\dagger})^n \varphi_0$ is normalized as well?

Just saying that $(\hat{a}^{\dagger})^n \varphi_0 = \left(\frac{1}{\sqrt{2}}\right)^n \left(\frac{1}{\sqrt{\pi}}\right)^{\frac{1}{2}} \left(\xi - \frac{\partial}{\partial \xi}\right)^n e^{-\left(\frac{\xi^2}{2}\right)}$,

$A_n \left(\xi - \frac{\partial}{\partial \xi}\right)^n e^{-\left(\frac{\xi^2}{2}\right)} = A_n \mathcal{H}_n(\xi)\, e^{-\left(\frac{\xi^2}{2}\right)} = \varphi_n$, $A_n = (2^n n! \sqrt{\pi})^{-\frac{1}{2}}$

$\rightarrow (2^n \sqrt{\pi})^{-\frac{1}{2}} \neq A_n$, What is the origin for $(n!)^{-\frac{1}{2}}$?

where A_1 is the normalization constant of φ_1. The nth eigenstate is given by the formula

$$\varphi_n = A_n\left(\xi - \frac{\partial}{\partial\xi}\right)^n e^{-\xi^2/2} \tag{7.57}$$

2 The nth-order differential operator $(\hat{a}^\dagger)^n$, when acting on the exponential form $\exp(-\xi^2/2)$, reproduces the same exponential factor, multiplied by an nth-order polynomial in ξ.

$$\left(\xi - \frac{\partial}{\partial\xi}\right)^n e^{-\xi^2/2} = \mathscr{H}_n(\xi)e^{-\xi^2/2} \tag{7.58}$$

Thus the nth eigenstate of the simple harmonic oscillator Hamiltonian may be written together with its eigenvalue as

$$\boxed{\begin{aligned} \varphi_n &= A_n\mathscr{H}_n(\xi)e^{-\xi^2/2} \\ E_n &= \hbar\omega_0(n + \tfrac{1}{2}) \end{aligned}} \tag{7.59}$$

3 The nth-order polynomials $\mathscr{H}_n(\xi)$ are well-known functions in mathematical physics. They are called *Hermite polynomials*. From (7.56) we see that $\mathscr{H}_1 = 2\xi$. The first six Hermite polynomials are listed in Table 7.1.

TABLE 7.1 The first six eigenenergies and eigenstates of the simple harmonic oscillator Hamiltonian

n	E_n	φ_n
0	$\hbar\omega_0/2$	$A_0 e -^{\xi^2/2}$
1	$3\hbar\omega_0/2$	$A_1 2\xi e^{-\xi^2/2}$
2	$5\hbar\omega_0/2$	$A_2(4\xi^2 - 2)e^{-\xi^2/2}$
3	$7\hbar\omega_0/2$	$A_3(8\xi^3 - 12\xi)e^{-\xi^2/2}$
4	$9\hbar\omega_0/2$	$A_4(16\xi^4 - 48\xi^2 + 12)e^{-\xi^2/2}$
5	$11\hbar\omega_0/2$	$A_5(32\xi^5 - 160\xi^3 + 120)e^{-\xi^2/2}$
		$A_n = (2^n n!\sqrt{\pi})^{-1/2}$

The nth-order Hermite polynomial $\mathscr{H}_n$ enters in the eigenfunctions φ_n of the quantum mechanical harmonic oscillator as

$$\varphi_n(\xi) = A_n\mathscr{H}_n(\xi)e^{-\xi^2/2}$$

$\mathscr{H}_n$ is a solution to *Hermite's equation*,

$$\mathscr{H}_n'' - 2\xi\mathscr{H}_n' + 2n\mathscr{H}_n = 0$$

2 The formulas connecting φ_n and φ_{n+1} (see Problem 7.9) are very useful in many problems relating to the simple harmonic oscillator. In Dirac notation they appear as

$$\begin{aligned} \hat{a}|\varphi_n\rangle &= n^{1/2}|\varphi_{n-1}\rangle \\ \hat{a}^{\dagger}|\varphi_n\rangle &= (n+1)^{1/2}|\varphi_{n+1}\rangle \end{aligned} \tag{7.60}$$

In place of $|\varphi_n\rangle$, let us write the ket vector $|n\rangle$. In this notation the equations above appear as

$$\begin{aligned} \hat{a}|n\rangle &= n^{1/2}|n-1\rangle \\ \hat{a}^{\dagger}|n\rangle &= (n+1)^{1/2}|n+1\rangle \end{aligned} \tag{7.61}$$

1 Let us check that

$$\hat{N}|n\rangle = n|n\rangle \tag{7.62}$$

With the aid of (7.61), we obtain

$$\begin{aligned} \hat{a}^{\dagger}\hat{a}|n\rangle &= \hat{a}^{\dagger}n^{1/2}|n-1\rangle = n^{1/2}n^{1/2}|n\rangle \\ \hat{a}^{\dagger}\hat{a}|n\rangle &= \hat{N}|n\rangle = n|n\rangle \end{aligned} \tag{7.63}$$

2 Inasmuch as $\{\varphi_n\}$ are normalized and are eigenstates of a Hermitian operator, they comprise an orthonormal sequence.

$$\int_{-\infty}^{\infty} \varphi_n{}^*\varphi_l \, d\xi = \langle n|l\rangle = \delta_{nl} \tag{7.64}$$

3 To gain familiarity with the manner in which these concepts are used in problems, we will work out a few illustrative examples.

First, consider the question: What is $\langle x\rangle$ in the nth eigenstate φ_n? Here we must calculate

$$\begin{aligned} \langle x\rangle &= \langle n|\hat{x}|n\rangle \\ &= \frac{1}{\sqrt{2\beta}}\langle n|\hat{a} + \hat{a}^{\dagger}|n\rangle \\ &= \frac{1}{\sqrt{2\beta}}\{n^{1/2}\langle n|n-1\rangle + (n+1)^{1/2}\langle n|n+1\rangle\} \\ &= 0 \end{aligned} \tag{7.65}$$

1 The last step follows from the orthogonality relation (7.64). The fact that the average value of x in any eigenstate φ_n vanishes is a consequence of the symmetry of the probability density $P = |\varphi_n|^2$ about the origin (see Fig. 7.10).

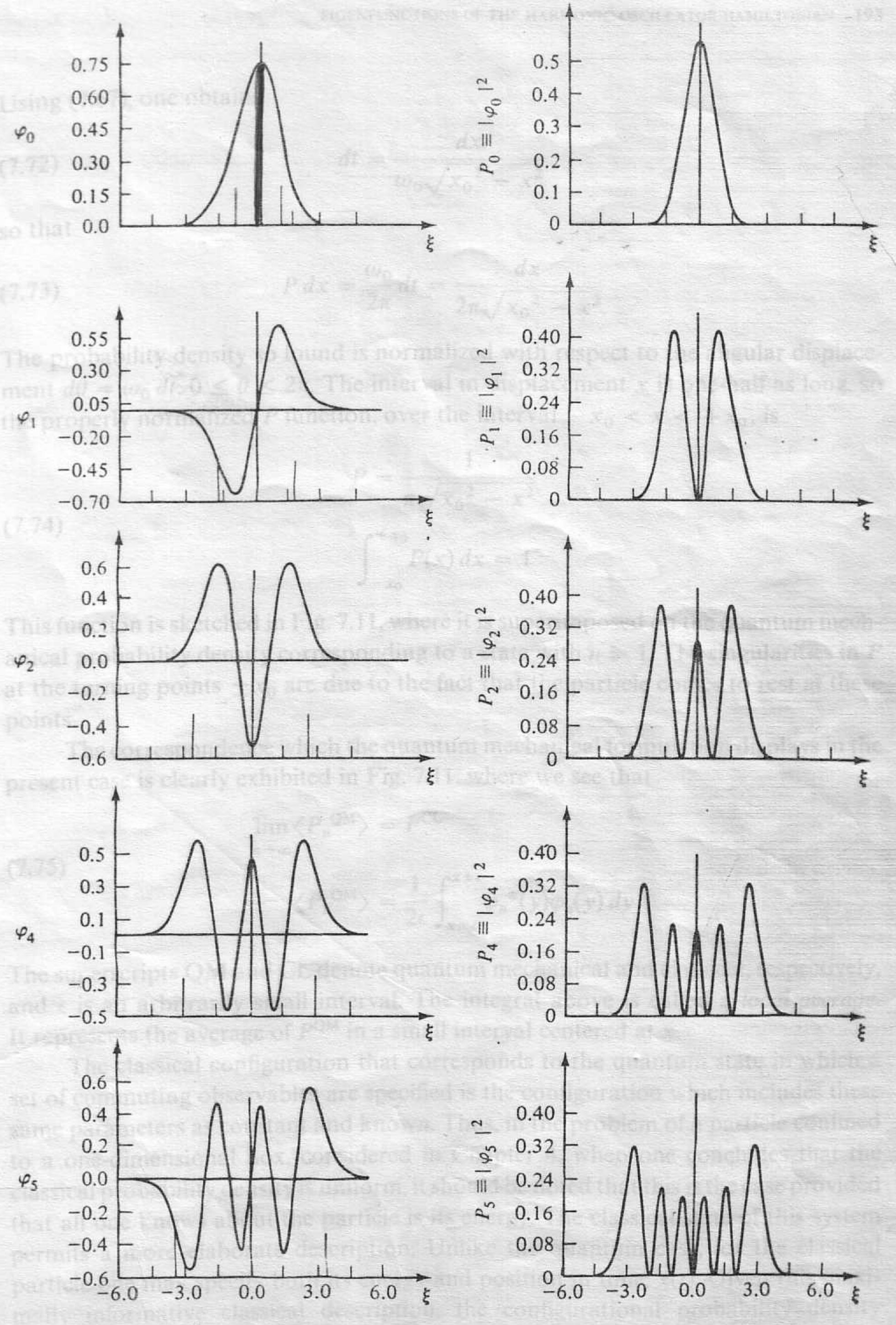

FIGURE 7.10 **The first six eigenstates of the simple harmonic oscillator and corresponding probability**

2 The second example we consider is the expectation of momentum p, in the nth eigenstate φ_n.

$$\langle p \rangle = \langle n|\hat{p}|n\rangle = \frac{m\omega_0}{\sqrt{2}i\beta}\langle n|\hat{a} - \hat{a}^\dagger|n\rangle \tag{7.66}$$

$$= \frac{m\omega_0}{\sqrt{2}i\beta}\{n^{1/2}\langle n|n-1\rangle - (n+1)^{1/2}\langle n|n+1\rangle\}$$

$$= 0$$

3 In any eigenstate φ_n of the Hamiltonian of the simple harmonic oscillator, the proba-
bility of finding the particle with momentum $\hbar k$ is equal to that of finding the particle
† 3. with momentum $-\hbar k$. Were we to express $\varphi_n(x)$ as a superposition of momentum
eigenstates, $\exp(ikx)$, we would find the probability amplitude $b(k)$ to be an even
(symmetric) function of k [i.e., $b(k) = b(-k)$].

Correspondence Principle

Next, we consider the manner in which the solution to the quantum mechanical harmonic oscillator problem obeys the *correspondence principle.* To these ends let us calculate the classical probability density P, corresponding to a one-dimensional spring with natural frequency ω_0. Let the particle be at the origin at $t = 0$ with velocity $x_0\omega_0$. The displacement at the time t is then given by

$$\begin{aligned} x &= x_0 \sin(\omega_0 t) \\ \dot{x} &= x_0\omega_0 \cos(\omega_0 t) \end{aligned} \tag{7.67}$$

This gives the correct initial data

$$\begin{aligned} x(0) &= 0 \\ \dot{x}(0) &= x_0\omega_0 \end{aligned} \tag{7.68}$$

The product $P(x)\,dx$ is the probability of finding the particle in the interval dx about the point x at any time. If T_0 is the period of oscillation

$$T_0 = \frac{2\pi}{\omega_0} \tag{7.69}$$

then

$$P\,dx = \frac{dt}{T_0} = \frac{\omega_0\,dt}{2\pi} \tag{7.70}$$

where

$$dt = \frac{dx}{\dot{x}} \tag{7.71}$$

Using (7.67), one obtains

$$dt = \frac{dx}{\omega_0\sqrt{{x_0}^2 - x^2}} \tag{7.72}$$

so that

$$P\,dx = \frac{\omega_0}{2\pi}\,dt = \frac{dx}{2\pi\sqrt{{x_0}^2 - x^2}} \tag{7.73}$$

The probability density so found is normalized with respect to the angular displacement $d\theta = \omega_0\,dt$, $0 \leq \theta \leq 2\pi$. The interval in displacement x is one-half as long, so the properly normalized P function, over the interval $-x_0 < x < +x_0$, is

$$\begin{gathered} P = \frac{1}{\pi\sqrt{{x_0}^2 - x^2}} \\ \int_{-x_0}^{+x_0} P(x)\,dx = 1 \end{gathered} \tag{7.74}$$

This function is sketched in Fig. 7.11, where it is superimposed on the quantum mechanical probability density corresponding to a state with $n \gg 1$. The singularities in P at the turning points $\pm x_0$ are due to the fact that the particle comes to rest at these points.

The correspondence which the quantum mechanical formulation displays in the present case is clearly exhibited in Fig. 7.11, where we see that

$$\begin{gathered} \lim_{n \to \infty} \langle {P_n}^{\text{QM}} \rangle = P^{\text{CL}} \\ \langle {P_n}^{\text{QM}} \rangle = \frac{1}{2\epsilon} \int_{x-\epsilon}^{x+\epsilon} \varphi_n{}^*(y)\varphi_n(y)\,dy \end{gathered} \tag{7.75}$$

The superscripts QM and CL denote quantum mechanical and classical, respectively, and ϵ is an arbitrarily small interval. The integral above is called a *local average*. It represents the average of P^{QM} in a small interval centered at x.

The classical configuration that corresponds to the quantum state in which a set of commuting observables are specified is the configuration which includes these same parameters as constant and known. Thus, in the problem of a particle confined to a one-dimensional box, considered in Chapter 4, when one concludes that the classical probability density is uniform, it should be noted that this is the case provided that all one knows about the particle is its energy. The classical state of this system permits a more elaborate description. Unlike the quantum case, for the classical particle one may specify both its energy and position in time, $x(t)$. Given this maximally informative classical description, the configurational probability density

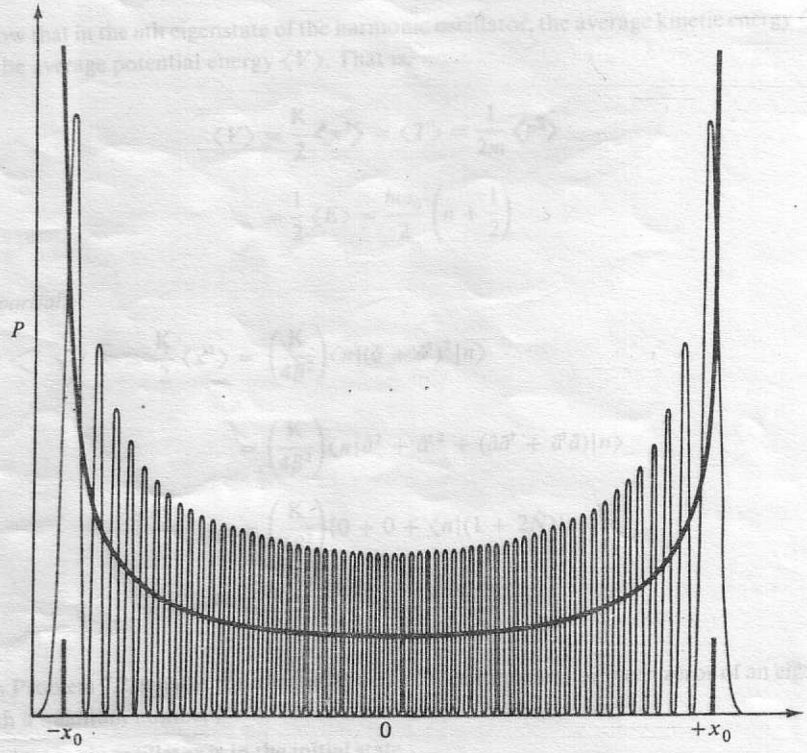

FIGURE 7.11 Classical probability density

$$P^{\mathrm{CL}} = \frac{1}{\pi\sqrt{{x_0}^2 - x^2}}$$

superimposed on the quantum mechanical probability density

$$P_n{}^{\mathrm{QM}} = |\varphi_n|^2$$

For the case $n \gg 1$,

$$\lim_{n\to\infty} \langle P_n{}^{\mathrm{QM}} \rangle = P^{\mathrm{CL}}$$

becomes $\delta[x(t) - x]$. When one speaks of configurational correspondence in the limit of high quantum numbers, what is usually meant is that in this limit the quantum probability density goes to the classical probability density in which, consistent with the quantum description, not more than the energy is specified.

In our consideration of correspondence for the harmonic oscillator, this rule is again obeyed. The expression (7.74) for the classical probability density is relevant

(7.8) $\varphi_n = A_n\left(\xi - \frac{\partial}{\partial\xi}\right) e^{-\left(\frac{\xi^2}{2}\right)}$, $\hat{P} f(x) = f(-x)$

$\rightarrow \hat{P}\varphi_n(\xi) = \varphi_n(-\xi) =$

$A_n\left((-\xi) - \frac{\partial}{\partial(-\xi)}\right)^n e^{-\left(\frac{(-\xi)^2}{2}\right)} =$

$A_n\left((-)\left(\xi - \frac{\partial}{\partial\xi}\right)\right)^n e^{-\xi^2/2} = (-)^n \varphi_n$

(7.9) (b) $\hat{a}\varphi_n = \hat{a}\left((n!)^{-\frac{1}{2}}\right)(\hat{a}^+)^n \varphi_0 =$

$(n)^{-\frac{1}{2}}((n-1)!)^{-\frac{1}{2}}(\hat{a}\hat{a}^+)((\hat{a}^+)^{n-1}\varphi_0 =>$, $\hat{a}\hat{a}^+ - \hat{a}^+\hat{a} = 1$

$\Rightarrow (n)^{-\frac{1}{2}}(1 + \hat{a}^+\hat{a})\left(((n-1)!)^{-\frac{1}{2}}(\hat{a}^+)^{n-1}\varphi_0\right) =$

$(n)^{-\frac{1}{2}}(1 + \hat{N})\varphi_{n-1} = (n)^{-\frac{1}{2}}(\cancel{1} + n - \cancel{1})\varphi_{n-1} =$

$(n)^{-\frac{1}{2}} n^{+\frac{1}{2}} n^{+\frac{1}{2}} \varphi_{n-1} = n^{\frac{1}{2}}\varphi_{n-1}$

(b)' $\hat{a}^+\varphi_n = (n!)^{-\frac{1}{2}}\hat{a}^+(\hat{a}^+)^n\varphi_0 =$

$(n+1)^{+\frac{1}{2}}(n+1)^{-\frac{1}{2}}((n)!)^{-\frac{1}{2}}(\hat{a}^+)^{n+1}\varphi_0 =$

$(n+1)^{\frac{1}{2}}((n+1)!)^{-\frac{1}{2}}(\hat{a}^+)^{n+1}\varphi_0 = (n+1)^{\frac{1}{2}}\varphi_{n+1}$

$\hat{a}|n\rangle = \sqrt{n}\,|n\rangle$, $\hat{a}^+|n\rangle = \sqrt{n+1}\,|n+1\rangle$

to the case where only the amplitude x_0, or equivalently the energy $E = Kx_0^2/2$, is known. The quantum density sketched in Fig. 7.11 is likewise connected to the energy eigenstate φ_n for which measurement of energy finds with certainty the value E_n.

PROBLEMS

7.6 (a) Show that the Hermite polynomials generated in the Taylor series expansion

$$\exp(2\xi t - t^2) = \sum_{n=0}^{\infty} \frac{\mathscr{H}_n(\xi)}{n!} t^n$$

are the same as generated in (7.58).

(b) Show that $\mathscr{H}_n$ as generated by

$$\mathscr{H}_n(\xi) = (-1)^n \left(e^{\xi^2} \frac{\partial^n}{\partial \xi^n} e^{-\xi^2} \right)$$

are equivalent to those given by (7.58).

(c) Use any of the preceding relations to establish

$$\mathscr{H}_n' = 2n\mathscr{H}_{n-1}$$

(d) and the recursion relation

$$\mathscr{H}_{n+1} = 2\xi\mathscr{H}_n - 2n\mathscr{H}_{n-1}$$

(e) Use the generating formula of part (b) to find $\mathscr{H}_0(\xi)$, $\mathscr{H}_1(\xi)$, and $\mathscr{H}_2(\xi)$.

7.7 The general formula for the normalization constant of φ_n is

$$A_n = (2^n n! \sqrt{\pi})^{-1/2}$$

Show that this gives correct normalization for φ_4.

7.8 Show directly from the form of φ_n given by (7.57) that

$$\hat{\mathbb{P}}\varphi_n = (-)^n \varphi_n$$

where $\hat{\mathbb{P}}$ is the parity operator.

7.9 (a) Show that the normalized nth eigenstate φ_n is generated from the normalized ground state φ_0 through

$$\varphi_n = \frac{1}{\sqrt{n!}} (\hat{a}^\dagger)^n \varphi_0$$

(b) Show that part (a) implies the following relations.

$$\hat{a}\varphi_n = n^{1/2}\varphi_{n-1}$$
$$\hat{a}^\dagger \varphi_n = (n+1)^{1/2}\varphi_{n+1}$$

where φ_n, φ_{n-1}, and φ_{n+1} are all normalized.

7.10 Show that in the nth eigenstate of the harmonic oscillator, the average kinetic energy $\langle T\rangle$ is equal to the average potential energy $\langle V\rangle$. That is,

$$\langle V\rangle = \frac{\mathrm{K}}{2}\langle x^2\rangle = \langle T\rangle = \frac{1}{2m}\langle p^2\rangle$$

$$= \frac{1}{2}\langle E\rangle = \frac{\hbar\omega_0}{2}\left(n+\frac{1}{2}\right)$$

Answer (partial)

$$< V >= \frac{\mathrm{K}}{2}\langle x^2\rangle = \left(\frac{\mathrm{K}}{4\beta^2}\right)\langle n|(\hat{a}+\hat{a}^\dagger)^2|n\rangle$$

$$= \left(\frac{\mathrm{K}}{4\beta^2}\right)\langle n|\hat{a}^2+\hat{a}^{\dagger 2}+(\hat{a}\hat{a}^\dagger+\hat{a}^\dagger\hat{a})|n\rangle$$

$$= \left(\frac{\mathrm{K}}{4\beta^2}\right)\{0+0+\langle n|(1+2\hat{N})|n\rangle\}$$

$$\langle V\rangle = \frac{\hbar\omega_0}{4}(1+2n) = \frac{\hbar\omega_0}{2}\left(n+\frac{1}{2}\right)$$

7.11 In Problem 7.2, what is the average spacing (in centimeters) between zeros of an eigenstate with such a quantum number?

7.12 A harmonic oscillator is in the initial state

$$\psi(x,0) = \varphi_n(x)$$

that is, an eigenstate of $\hat{H}$. What is $\psi_n(x,t)$?

7.13 For a harmonic oscillator in the superposition state

$$\psi(x,t) = \frac{1}{\sqrt{2}}[\psi_0(x,t)+\psi_1(x,t)]$$

show that

$$\langle x\rangle = C\cos(\omega_0 t)$$

In the notation above,

$$\psi_n(x,t) \equiv \varphi_n(x)\exp\left(-\frac{iE_n t}{\hbar}\right)$$

7.14 Show that in the nth state of the harmonic oscillator,

$$\langle x^2\rangle = (\Delta x)^2$$

$$\langle p^2\rangle = (\Delta p)^2$$

7.15 Find $\langle x \rangle$ for a harmonic oscillator in the superposition state

$$\psi(x, t) = \frac{1}{\sqrt{2}} [\psi_0(x, t) + \psi_3(x, t)]$$

The harmonic oscillator has natural frequency ω_0.

7.16 A large dielectric cube with edge length L is uniformly charged throughout its volume so that it carries a total charge Q. It fills the space between condenser plates, which have a potential difference Φ_0 across them. An electron is free to move in a small canal drilled in the dielectric normal to the plates (Fig. 7.12).

The Hamiltonian for the electron is

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{\mathrm{K}x^2}{2} + \frac{e\Phi_0}{L} x$$

(a) What is the spring constant K in terms of the total charge Q?

(b) What are the eigenenergies and eigenfunctions of $\hat{H}$? [*Hint:* Rewrite the potential energy of the electron as

$$V = \frac{\mathrm{K}}{2}(x^2 + 2\gamma x) = \frac{\mathrm{K}}{2}[(x + \gamma)^2 - \gamma^2]$$

$$\gamma \equiv \frac{e\Phi_0}{L\mathrm{K}}$$

then change variables to $z \equiv x + \gamma$. To evaluate K, use Gauss's law (neglecting "edge effects").]

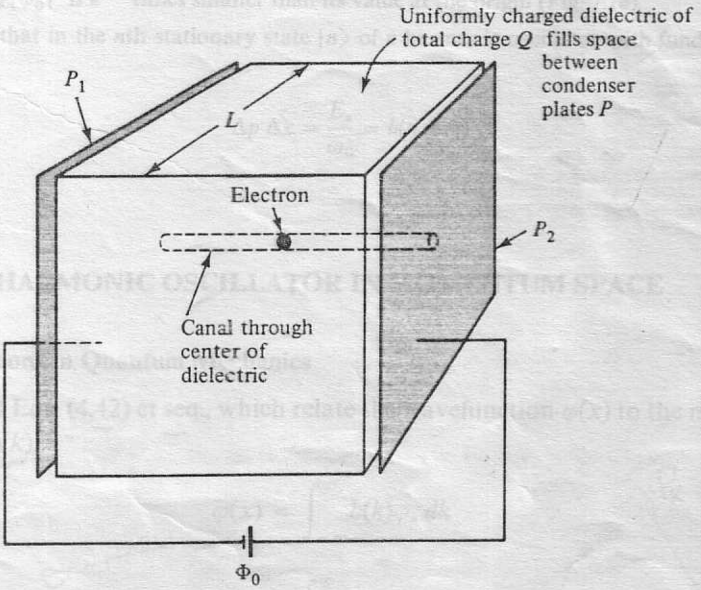
Uniformly charged dielectric of total charge Q fills space between condenser plates P
P_1
L
Electron
P_2
Canal through center of dielectric
Φ_0

FIGURE 7.12 Configuration described in Problem 7.16.

7.17 (a) Show that the time-independent Schrödinger equation for the harmonic oscillator, with the energy eigenvalues (7.44), may be written

$$\varphi_{\xi\xi} + (2n + 1 - \xi^2)\varphi = 0$$

(b) Using the relations of Problem 7.6, show that

$$\varphi_n = \mathscr{H}_n(\xi)e^{-\xi^2/2}$$

is a solution to this equation.

(c) Obtain Hermite's equation

$$\mathscr{H}_n'' - 2\xi\mathscr{H}_n' + 2n\mathscr{H}_n = 0$$

7.18 Use the uncertainty principle between x and p to derive the "zero-point" energy

$$E_0 = \tfrac{1}{2}\hbar\omega_0$$

of a harmonic oscillator with natural frequency ω_0 (see Fig. 7.8).

$\Delta x \Delta p \simeq \frac{\hbar}{2} \to$ ①

$\Delta x = \sqrt{\langle x^2 \rangle}$

$\Delta p = \sqrt{\langle p^2 \rangle}$

$\Delta x \Delta p = \frac{E_n}{\omega_0}$ for zer $n=0$

$\frac{E_0}{\omega_0} = \frac{\hbar}{2} \to E_0 = \frac{1}{2}\hbar\omega_0$

7.19 Show that

$$\hat{a}^\dagger\hat{a} = \frac{1}{2}\left(\xi^2 - \frac{\partial^2}{\partial\xi^2} - 1\right)$$

in the nondimensional ξ notation.

7.20 Show that the asymptotic exponential behavior of $\varphi_n(\xi)$ agrees with that obtained directly from the Schrödinger equation, in the limit that $\xi \to \infty$.

7.21 Show that

$$\left(\xi + \frac{\partial}{\partial\xi}\right)^\dagger = \xi - \frac{\partial}{\partial\xi}$$

in $\mathfrak{H}_2$ (see Eq. 4.31).

7.22 (a) What is the asymptotic solution φ_n to the Schrödinger equation (as given in Problem 7.17)

$$\varphi_{\xi\xi} + (2n + 1 - \xi^2)\varphi = 0$$

in the domain

$$\xi^2 \ll 1 + 2n \simeq 2n?$$

(b) Show that

$$\lim_{n \gg 1} \langle P_n \rangle = \langle |\tilde{\varphi}_n|^2 \rangle = \text{constant}$$

Answer

In this domain the Schrödinger equation above becomes

$$\tilde{\varphi}_{\xi\xi} + 2n\tilde{\varphi} = 0$$

which has the (even) solution

$$\tilde{\varphi}_n = C\cos(\sqrt{2n}\,\xi)$$

It follows that the local average of $|\tilde{\varphi}_n|^2$ in this domain is given by

$$\langle|\tilde{\varphi}_n|^2\rangle = \frac{C^2}{2\epsilon}\int_{\xi-\epsilon}^{\xi+\epsilon}\cos^2(\sqrt{2n}\,\xi)\,d\xi$$

$$= \frac{C^2}{2\epsilon}\left\{\epsilon + \frac{1}{2\sqrt{2n}}[\sin(2\sqrt{2n}\epsilon)\cos(2\sqrt{2n}\,\xi)]\right\}$$

$$\lim_{n\to\infty}\langle P_n\rangle = \frac{C^2}{2}$$

(1) This result explains the flatness of $\langle P^{QM}\rangle$ in the central domain $\xi^2 \ll 2n$, as seen in Fig. 7.11.

7.23 Estimate the length of interval about $x = 0$ which corresponds to the classically allowed domain for the ground state of the simple harmonic oscillator.

Answer

The turning points occur at

$$\xi = \pm 1 \quad \text{or equivalently at} \quad x = \pm\sqrt{\frac{\hbar}{m\omega_0}} \quad =$$

At this value, $|\varphi_0|^2$ is e^{-1} times smaller than its value at the origin (Fig. 7.10).

7.24 Show that in the nth stationary state $|n\rangle$ of a harmonic oscillator with fundamental frequency ω_0,

$$\Delta p\,\Delta x = \frac{E_n}{\omega_0} = \hbar(n+\tfrac{1}{2})$$

7.4 THE HARMONIC OSCILLATOR IN MOMENTUM SPACE

Representations in Quantum Mechanics

Let us recall Eqs. (4.42) et seq., which relate the wavefunction $\varphi(x)$ to the momentum coefficient $b(k)$.

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$$\varphi(x) = \int_{-\infty}^{\infty} b(k)\varphi_k\,dk$$

(7.76)

$$b(k) = \int_{-\infty}^{\infty} \varphi(x)\varphi_k{}^*\,dx \quad = \quad \langle\varphi|\varphi_k\rangle$$

$\varphi_k = \frac{1}{\sqrt{3\pi}}e^{ikx}$

e. f of $\hat{P}$

$\varphi(x)$ any element $\in \mathcal{H}_1$

The eigenfunction of momentum corresponding to the value $p = \hbar k$ is φ_k. The wavefunction $\varphi(x)$ gives the probability density in coordinate space through the Born relation

$$P(x) = |\phi(x)|^2 \tag{7.77}$$

The momentum coefficient $b(k)$ gives the probability density [probability of finding the particle to have momentum in the interval $\hbar k$ to $\hbar(k + dk)$] in momentum (k) space through the relation

$$P(k) = |b(k)|^2 \tag{7.78}$$

2 The integral formulas (7.76) serve to determine $\varphi(x)$ given $b(k)$, and vice versa. It follows that any information contained in $\varphi(x)$ can be obtained from knowledge of $b(k)$ and vice versa. Given the Hamiltonian of a system, $\varphi(x)$ is determined. Let us construct an equation which similarly determines $b(k)$ from the Hamiltonian [i.e., without first finding $\varphi(x)$]. To these ends we first recall the time-independent Schrödinger equation for the harmonic oscillator.

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{\mathrm{K}x^2}{2}\right)\varphi(x) = E\varphi(x) \tag{7.79}$$

2 Substituting the Fourier decomposition of $\varphi(x)$ above and noting the equality

$$x\varphi_k = +i\frac{\partial \varphi_k}{\partial k} \tag{7.80}$$

gives

$$\int_{-\infty}^{\infty} dk b(k)\left(\frac{\hbar^2 k^2}{2m} - \frac{\mathrm{K}}{2}\frac{\partial^2}{\partial k^2}\right)\varphi_k = E\int_{-\infty}^{\infty} dk b(k)\varphi_k \tag{7.81}$$

3 Integrating the second term on the left-hand side by parts twice and setting

$$b(k)|_{k=\pm\infty} = 0 \tag{7.82}$$

gives

$$\int_{-\infty}^{\infty} dk\varphi_k\left[\left(\frac{\hbar^2 k^2}{2m} - \frac{\mathrm{K}}{2}\frac{\partial^2}{\partial k^2} - E\right)b(k)\right] = 0 \tag{7.83}$$

2 It follows that the term in brackets is the Fourier transform of zero, which is zero. We conclude that $b(k)$ (appropriate to the harmonic oscillator) satisfies the *k-dependent Schrödinger equation*

$$\left(\frac{\hbar^2 k^2}{2m} - \frac{\mathrm{K}}{2}\frac{\partial^2}{\partial k^2}\right)b(k) = Eb(k) \tag{7.84}$$

This equation is also called the *Schrödinger equation in momentum representation.*

1 We note that the Hamiltonian in momentum representation includes the simple multiplicative operator $\hbar k$ in place of p and the differential operator $+i\partial/\partial k$ in place
2 of x. This rule for obtaining the structure of the Hamiltonian in momentum representation always holds providing the potential $V(x)$ is an analytic function[1] of x (i.e., has a well-defined power-series expansion). For such cases the Schrödinger equation in either coordinate or momentum space is obtained through the recipes:

$$\text{In } x\text{-space:}\quad \hat{H}(x, p) \rightarrow \hat{H}\left(x, -\frac{i\hbar\,\partial}{\partial x}\right)$$

$$\text{In } p\text{-space:}\quad \hat{H}(x, p) \rightarrow \hat{H}\left(+\frac{i\partial}{\partial k}, \hbar k\right)$$

$$\varphi(x) \rightarrow b(k)$$

·3 The time-dependent Schrödinger equation in momentum representation appears as

$$i\hbar\frac{\partial}{\partial t}b(k, t) = \hat{H}(k)b(k, t) \tag{7.85}$$

1 Paralleling the development of (3.70) permits the solution to (7.85) for the initial-value problem for $b(k, t)$ to be written

$$b(k, t) = \exp\left(-\frac{it\hat{H}}{\hbar}\right)b(k, 0) \tag{7.86}$$

2 For free-particle motion with $\hat{H} = \hbar^2k^2/2m$, the latter relation gives

$$|b(k, t)|^2 = |b(k, 0)|^2 \tag{7.87}$$

The momentum probability density for free-particle motion is constant in time.

3 Geometrically, the function $b(k)$ is the projection of the state $\varphi(x)$ onto the momentum eigenstate φ_k (recall Eq. 4.44).

$$b(k) = \langle\varphi_k|\varphi\rangle \tag{7.88}$$

· For any given state $\varphi(x)$, the function $b(k)$ represents a distribution of values, corresponding to the projections of $\varphi(x)$ onto the set of basis vectors $\{\varphi_k\}$. The functions
3· $b(k)$ and $\varphi(x)$ are equally informative. In momentum representation a state of the system is represented by its projections onto the basis of Hilbert space $\{\varphi_k\}$. (See Fig. 4.6.)

1· This is analogous to the statement that a vector $\mathbf{B}$ in 3-space is represented by its projections onto the three unit vectors $\mathbf{e}_x$, $\mathbf{e}_y$, and $\mathbf{e}_z$, namely B_x, B_y, and B_z.

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† [1] In the more general case the Schrödinger equation in momentum space becomes an integral equation. These topics are discussed in greater detail in E. Merzbacher, *Quantum Mechanics*, 2nd ed., Wiley, New York, 1970.

These are not the only basis vectors one can use to represent the vector **B**. For instance, one can employ the basis $\mathbf{e}_x'$, $\mathbf{e}_y'$, and $\mathbf{e}_z'$ given by

$$\mathbf{e}_x' = \frac{1}{\sqrt{2}}(\mathbf{e}_x + \mathbf{e}_y)$$

$$\mathbf{e}_y' = \frac{1}{\sqrt{2}}(\mathbf{e}_x - \mathbf{e}_y) \tag{7.89}$$

$$\mathbf{e}_z' = \mathbf{e}_z$$

(See Fig. 7.13.) In this basis **B** is represented by the three components

$$\mathbf{B} = (B_x', B_y', B_z') = \frac{1}{\sqrt{2}}(B_x + B_y, B_x - B_y, \sqrt{2}B_z)$$

+ 1 There are countless other triads of unit vectors which are valid bases of 3-space (i.e., they all span 3-space). The three components of **B** in any one of these representations completely specify **B**.

Similarly, one may describe the state of a system in quantum mechanics in
different representations. In each of these, a distinct set of vectors serves as a basis of
1 Hilbert space. Particularly important in the theory of representations is the concept of
common eigenfunctions of some *complete set of commuting operators* relevant to a
2 given system. Suppose that the complete set of commuting operators are $\hat{A}$, $\hat{B}$, and $\hat{C}$.
In the state φ_{abc} (common eigenstates of $\hat{A}$, $\hat{B}$, and $\hat{C}$) one may specify the "good"
quantum numbers a, b, and c. The state of the system cannot be further resolved.
3 Such states may serve as a basis of Hilbert space. The representation in which all
states are referred to the basis $\{\varphi_{abc}\}$ is called the *abc representation*, just as we call

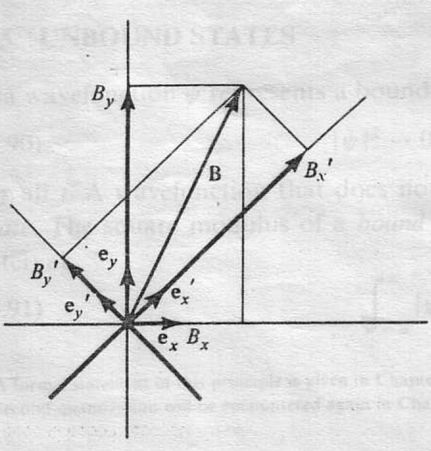

FIGURE 7.13 Projections onto two sets of basis vectors (in the xy plane) of the vector B. The two bases are related through (7.89). The z component is the same in both representations.

the representation in which states are referred to the eigenfunctions of momentum, the *momentum representation.*[1] One also speaks of the *abc* representation as the one in which $\hat{A}$, $\hat{B}$, and $\hat{C}$ are *diagonal.*

PROBLEMS

7.25 Show that $b(k)$ is even for any even potential $V(x) = V(-x)$. What can be concluded about the oddness or evenness of $b(k)$ if $V(x)$ is an odd function, $V(x) = -V(-x)$?

7.26 What are the eigenfunctions $b_n(k)$ of the harmonic oscillator Hamiltonian $\hat{H}(k)$ in momentum space (as given by Eq. 7.84)? [*Hint:* Note the similarity between $\hat{H}(k)$ and $\hat{H}(x)$, and the boundary conditions of $\varphi_n(x)$ and $b_n(k)$.]

7.27 What is the Schrödinger equation in momentum representation for a free particle moving in one dimension? What are the eigenfunctions $b(k)$ of this equation?

7.28 Consider the Gaussian wave packet whose initial momentum probability density is given by (6.45).

(a) What is $|b(k, t)|^2$ at $t > 0$?

(b) What is $\Delta x \, \Delta p$ at $t > 0$?

7.29 Consider an arbitrary differentiable function of p, $\varphi(p)$. Show that with $\hat{p} = p$ and $\hat{x} = +i\hbar \, \partial/\partial p$,

$$[\hat{x}, \hat{p}]\varphi(p) = i\hbar\varphi(p)$$

7.30 What is the eigenfunction of the operator $\hat{x}$, in the momentum representation, corresponding to the eigenvalue x? That is, give the solution to the equation

$$\hat{x}\varphi_x(p) = x\varphi_x(p)$$

7.31 Let $|x'\rangle$ denote an eigenvector of the position operator $\hat{x}$ with eigenvalue x' and let $|k'\rangle$ denote an eigenvector of the momentum operator $\hat{p}$ with eigenvalue $\hbar k'$. Show that

(a) $\langle k|k'\rangle = \delta(k - k')$

(b) $\langle x|x'\rangle = \delta(x - x')$

(c) $\langle x|k\rangle = \dfrac{1}{\sqrt{2\pi}} \exp(ikx)$

For each case, state in which representation you are working.

7.32 Suppose that the operators $\hat{a}$ and $\hat{a}^\dagger$ in

$$\hat{H} = \hbar\omega_0(\hat{a}^\dagger\hat{a} + \tfrac{1}{2})$$

obey the *anticommutation* relation

$$\{\hat{a}, \hat{a}^\dagger\} \equiv \hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a} = 1$$

---

[1] For further discussion of the coordinate and momentum representations, see Appendix A.

(a) What are the values of $\hat{a}|n\rangle$ and $\hat{a}^\dagger|n\rangle$ that follow from the anticommutation relation above? [illegible]

(b) Since $\langle H\rangle \geq 0$, for consistency we may again set

$$\hat{a}|0\rangle = 0$$

Combining this fact with your answer to part (a), which are the only nonvanishing states $|n\rangle$?

(c) If, in addition to the anticommutation property above, $\hat{a}$ and $\hat{a}^\dagger$ also obey the relations, $\{\hat{a}, \hat{a}\} = \{\hat{a}^\dagger, \hat{a}^\dagger\} = 0$, show that $\hat{N}^2 = \hat{N}$.

Answer (partial)

(a) $\hat{a}|n\rangle = \sqrt{n}|1-n\rangle$

$\hat{a}^\dagger|n\rangle = \sqrt{1-n}|1-n\rangle$

(b) The only nonvanishing states are $|0\rangle$ and $|1\rangle$. [*Note:* Anticommutation relations between $\hat{a}$ and $\hat{a}^\dagger$ are used to describe particles that obey the *Pauli exclusion principle.*[1] In this context the operator $\hat{N}$ denotes the number of particles in a given state so that (b) implies that there is no more than one particle in any state. The $|0\rangle$ state is called the *vacuum state.* The formalism is known as *second quantization.*[2]]

7.33 What is the lowest value of kinetic energy $\langle T\rangle$ a harmonic oscillator with frequency ω_0 can have?

Answer

$\langle v\rangle = \langle T\rangle$

In Problem 7.10 we found that in the nth eigenstate of the oscillator

$$\langle V\rangle = \langle T\rangle = \frac{\hbar\omega_0}{2}\left(n + \frac{1}{2}\right) \geq \frac{\hbar\omega_0}{4}$$

Thus, the lowest allowed energy of the oscillator is $\hbar\omega_0/2$. It is impossible to force the oscillator to a lower energy. In a solid, for example, whose nuclei are bound together by harmonic forces, this zero-point energy persists at 0 K. (See Problem 7.18.)

$\hbar\omega_0/2$

$\hbar\omega_0/2$

7.5 UNBOUND STATES

If a wavefunction ψ represents a bound state (in one dimension), then

$$|\psi|^2 \to 0, \qquad |x| \to \infty \tag{7.90}$$

for all t. A wavefunction that does not obey this condition represents an *unbound state*. The square modulus of a *bound state* gives a finite integral over the infinite interval.

$$\int_{-\infty}^{\infty} |\psi|^2\, dx < \infty \tag{7.91}$$

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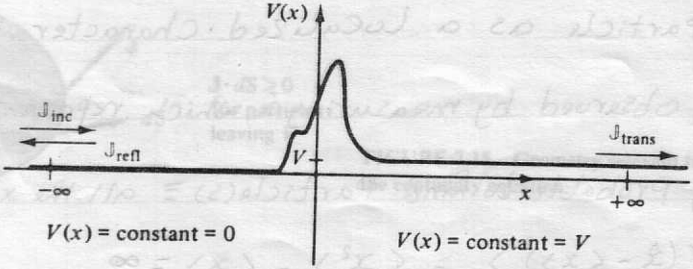
[1] A formal statement of this principle is given in Chapter 12. See also Appendix B.

[2] Second quantization will be encountered again in Chapter 13.



$V(x)$
$\mathbb{J}_{\text{inc}}$
$\mathbb{J}_{\text{refl}}$
$\mathbb{J}_{\text{trans}}$
V
$-\infty$
x
$+\infty$
$V(x) = \text{constant} = 0$
$V(x) = \text{constant} = V$

FIGURE 7.14 **One-dimensional scattering problem. Incident particle current $\mathbb{J}_{\text{inc}}$ initiated at $x = -\infty$ is partially transmitted ($\mathbb{J}_{\text{trans}}$) and partially reflected ($\mathbb{J}_{\text{refl}}$) by a potential barrier $V(x)$. The potential is constant outside the scattering domain.**

1. The square modulus of an *unbound state* gives a finite integral over *any* finite interval.

(7.92)
$$\int_a^b |\psi|^2\,dx < \infty, \qquad |b-a| < \infty$$

2 → The eigenstate of the momentum operator

(7.93)
$$\varphi_n(x) = \frac{1}{\sqrt{2\pi}} e^{ikx}$$

2. represents an unbound state. The eigenfunction of the simple harmonic oscillator Hamiltonian

(7.94)
$$\varphi_n(\xi) = A_n \mathscr{H}_n(\xi) e^{-\xi^2/2}$$

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† 3 (see Section 7.3) represents a bound state. Unbound states are relevant to scattering problems. Such problems characteristically involve a beam of particles which is incident on a potential barrier (Fig. 7.14).

4 Since $\int_{-\infty}^{\infty} |\psi|^2\,dx$ diverges for unbound states, it is convenient to normalize the wavefunction for scattering problems in terms of the particle density ρ. For one-dimensional scattering problems we take

$$\star \qquad |\psi|^2\,dx = \rho\,dx = dN$$
$$= \text{number of particles in the interval } dx$$

(7.95)
$$\therefore \int_a^b |\psi|^2\,dx = N$$
$$= \text{number of particles in the interval } (b-a)$$

! For a one-dimensional beam of 10^3 neutrons/cm, all moving with momentum $p = \hbar k_0$, the wavefunction is written

$$\psi = 10^{3/2} e^{i(k_0 x - \omega t)}, \qquad |\psi|^2 = 10^3\ \text{cm}^{-1}$$

(7.96)
$$\frac{\hbar^2 k_0{}^2}{2m} = \hbar\omega$$

† 2 The sole difference between ψ so defined and a wavefunction whose square modulus is probability density is a multiplicative constant. It follows that $|\psi|^2$, when referred
2 to particle density, is proportional to probability density also. For uniform beams,
3 $|\psi|^2$ is constant, which in turn implies that it is uniformly probable to find particles
$(\Delta x = \infty)$ anywhere along the beam. This is consistent with the uncertainty principle. For instance, for the wavefunction (7.96), the momentum of any neutron in the beam is hk_0, whence its position is maximally uncertain.

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Continuity Equation

particle ~ probability

One-dimensional barrier problems involve incident, reflected, and transmitted *current densities*, $\mathbb{J}_{\text{inc}}$, $\mathbb{J}_{\text{refl}}$, and $\mathbb{J}_{\text{trans}}$, respectively. In three dimensions the number density and current density $\mathbf{J}$ are related through the *continuity equation*

(7.97) "apply in G space"
$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{J} = 0$$

! To clarify the physical meaning of this equation, we integrate it over a volume V and obtain

(7.98)
$$\int_v \frac{\partial \rho}{\partial t}\, dv = \frac{\partial N}{\partial t} = -\int_S \mathbf{J} \cdot d\mathbf{S} = -\int_v \nabla \cdot \underline{J}\, dv = \frac{\partial}{\partial t}\left(\int_v \rho\, dv\right)$$

The total number of particles in the volume V is

(7.99)
$$N = \int_V \rho\, d\tau$$

(Gauss's theorem was used to transform the divergence term.) The surface S encloses
2 the volume V (Fig. 7.15). Equation (7.98) says that the number of particles in the volume V changes by virtue of a net flux of particles out of (or into) the volume V.
† 2 It is a statement of the *conservation of matter* because it says that this is the *only* way the total number of particles in V can change. If particles are born spontaneously
3 in V with no net flux of particles through the surface S, then $\partial N/\partial t > 0$, while $\int \mathbf{J} \cdot d\mathbf{S} = 0$ and (7.98) is violated.

[illegible]

1 To find Particle(s) implies that we measure $\hat{x}$,

because a particle as a localized character is

best best observed by measuring $\hat{x}$ which represents localization

2 When: equally probable to find Particle(s) ≡ all the x's are the same.

i.e $(\Delta x)^2 = \langle (\hat{x} - \langle x \rangle)^2 \rangle = \langle x^2 \rangle - \langle x \rangle = \infty$

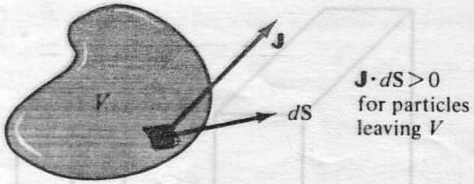


FIGURE 7.15 Geometry relevant to integration of the continuity equation.

If particles are moving only in the x direction,

$$\mathbf{J} = (\mathbb{J}_x, 0, 0) \tag{7.100}$$

and the continuity equation becomes

$$\frac{\partial \rho}{\partial t} + \frac{\partial \mathbb{J}_x}{\partial x} = 0 \tag{7.101}$$

1 We already have identified ρ with $|\psi|^2$. To relate $\mathbb{J}_x$ to ψ, we must construct an equation that looks identical to (7.101) with $|\psi|^2$ in place of ρ. Then the functional of ψ which appears after $\partial/\partial x$ is $\mathbb{J}_x$.

2 The wavefunction for particles in the beam obeys the Schrödinger equation

$$\frac{\partial \psi}{\partial t} = -\frac{i}{\hbar}\hat{H}\psi, \qquad \frac{\partial \psi^*}{\partial t} = +\frac{i}{\hbar}\hat{H}\psi^* \tag{7.102}$$

The time derivative of the particle density $\psi^*\psi$ is

$$\frac{\partial \psi^*\psi}{\partial t} = \psi^*\frac{\partial \psi}{\partial t} + \frac{\psi\,\partial \psi^*}{\partial t} = \psi^*\left(\frac{-i\hat{H}}{\hbar}\psi\right) + \psi\left(\frac{+i\hat{H}}{\hbar}\psi^*\right) \tag{7.103}$$

3 For the typical one-dimensional Hamiltonian

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(x) \tag{7.104}$$

the latter equation becomes

$$\begin{gathered} \frac{\partial \psi^*\psi}{\partial t} = \frac{i\hbar}{2m}(\psi^*\psi_{xx} - \psi\psi^*_{xx}) \\ \frac{\partial \psi^*\psi}{\partial t} + \frac{\partial}{\partial x}\left[\frac{\hbar}{2mi}\left(\psi^*\frac{\partial \psi}{\partial x} - \psi\frac{\partial \psi^*}{\partial x}\right)\right] = 0 \end{gathered} \tag{7.105}$$

3 (The subscript x denotes differentiation.) Comparison of this equation with (7.101) permits the identification

$$\mathbb{J}_x = \frac{\hbar}{2mi}\left(\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x}\right) \tag{7.106}$$

Note that the dimensions of $\mathbb{J}_x$ are number per second. In three dimensions the current density is written

$$\mathbf{J} = \frac{\hbar}{2mi}(\psi^* \nabla \psi - \psi \nabla \psi^*) \tag{7.107}$$

$\frac{\hbar}{2mi} = -i\frac{\hbar}{2m}$

and has dimensions $\text{cm}^{-2}\,\text{s}^{-1}$.

Transmission and Reflection Coefficients

1 For one-dimensional scattering problems, the particles in the beam are in plane-wave states with definite momentum. Given the wavefunctions relevant to incident, reflected, and transmitted beams, one may calculate the corresponding current densities according to (7.106). The *transmission coefficient* T and *reflection coefficient* R are defined as

$$T \equiv \left|\frac{\mathbb{J}_{\text{trans}}}{\mathbb{J}_{\text{inc}}}\right|, \qquad R \equiv \left|\frac{\mathbb{J}_{\text{refl}}}{\mathbb{J}_{\text{inc}}}\right| \tag{7.108}$$

2 These one-dimensional barrier problems are closely akin to problems on the transmission and reflection of electromagnetic plane waves through media of varying index of refraction (see Fig. 7.16). In the quantum mechanical case, the scattering is also of waves.

3 For one-dimensional barrier problems there are three pertinent beams. Particles in the incident beam have momentum

$$p_{\text{inc}} = \hbar k_1 \tag{7.109}$$

Particles in the reflected beam have the opposite momentum

$$p_{\text{refl}} = -\hbar k_1 \tag{7.110}$$

3 In the event that the environment (i.e., the potential) in the domain of the transmitted beam ($x = +\infty$) is different from that of the incident beam ($x = -\infty$), the momenta in these two domains will differ. Particles in the transmitted beam will have momentum $\hbar k_2 \neq \hbar k_1$,

$$p_{\text{trans}} = \hbar k_2 \tag{7.111}$$

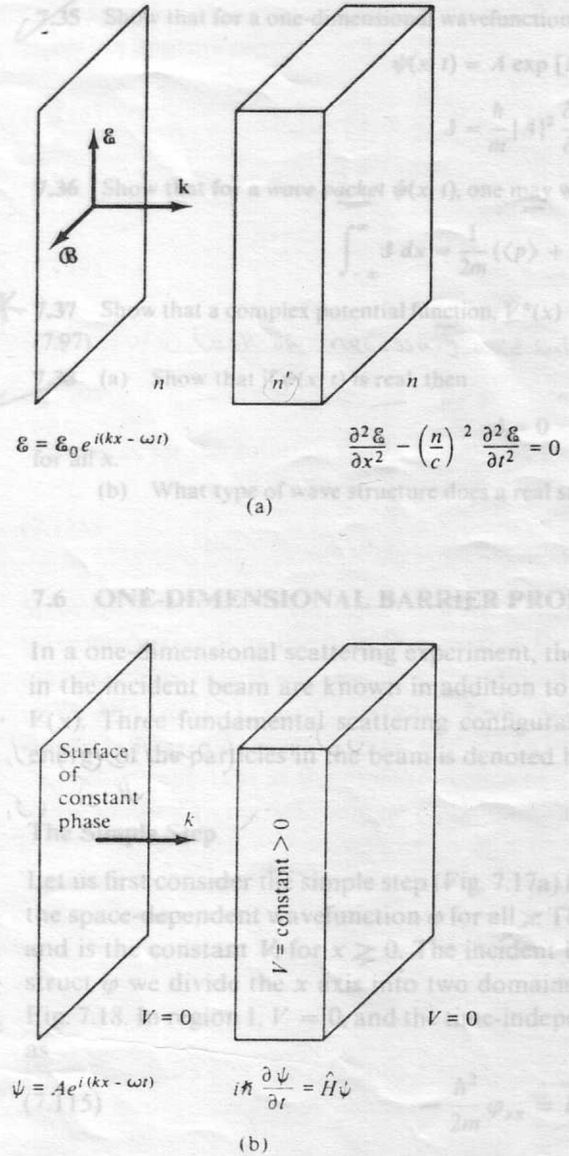

ℰ
k
ℬ
n
n'
n
$\mathcal{E} = \mathcal{E}_0 e^{i(kx - \omega t)}$
$\frac{\partial^2 \mathcal{E}}{\partial x^2} - \left(\frac{n}{c}\right)^2 \frac{\partial^2 \mathcal{E}}{\partial t^2} = 0$
(a)
Surface of constant phase
k
V = constant > 0
V = 0
V = 0
$\psi = Ae^{i(kx - \omega t)}$
$i\hbar \frac{\partial \psi}{\partial t} = \hat{H}\psi$
(b)

FIGURE 7.16 **(a) Scattering of plane electromagnetic waves through domains of different index of refraction *n*. (b) Scattering of plane, free-particle wavefunctions through domains of different potential.**

What is the Source for the Presence of the Potential ?

Scalar/Complex Potential

·1 In all cases the potential is constant in the domains of the incident and transmitted beams (see Fig. 7.14), so the wavefunctions in these domains describe free particles, and we may write

$$\text{(7.112)}\qquad \begin{aligned} \psi_{\text{inc}} &= Ae^{i(k_1x-\omega_1t)}, & \hbar\omega_1 &= E_{\text{inc}} = \frac{\hbar^2k_1{}^2}{2m} \\ \psi_{\text{refl}} &= Be^{-i(k_1x+\omega_1t)}, & \hbar\omega_1 &= E_{\text{refl}} = E_{\text{inc}} \\ \psi_{\text{trans}} &= Ce^{i(k_2x-\omega_2t)}, & \hbar\omega_2 &= E_{\text{trans}} = \frac{\hbar^2k_2{}^2}{2m} + V \\ & & &= E_{\text{inc}} = \hbar\omega_1 \end{aligned}$$

† 1 Energy is conserved across the potential hill so that frequency remains constant ($\omega_1 = \omega_2$). The change in wavenumber k corresponds to changes in momentum and 1· kinetic energy. Using (7.106) permits calculation of the currents

$$\text{(7.113)}\qquad \begin{aligned} \mathbb{J}_{\text{inc}} &= \frac{\hbar}{2mi}\,2ik_1|A|^2 \\ \mathbb{J}_{\text{trans}} &= \frac{\hbar}{2mi}\,2ik_2|C|^2 \\ \mathbb{J}_{\text{refl}} &= -\frac{\hbar}{2mi}\,2ik_1|B|^2 \end{aligned}$$

2 It should be noted that these relations are equivalent to the classical prescription for 3 particle current, $\mathbb{J} = \rho v$, with $\rho = |\psi|^2$ and $v = \hbar k/m$. These formulas, together with (7.108), give the T and R coefficients

$$\text{(7.114)}\qquad T = \left|\frac{C}{A}\right|^2\frac{k_2}{k_1}, \qquad R = \left|\frac{B}{A}\right|^2$$

In the event that the potentials in domains of incident and transmitted beams are 3· equal, $k_1 = k_2$ and $T = |C/A|^2$. More generally, to calculate C/A and B/A as functions of the parameters of the scattering experiment (namely, incident energy, structure of potential barrier), one must solve the Schrödinger equation across the domain of the potential barrier.

PROBLEMS

✓ **7.34** Show that the current density **J** may be written

$$\mathbf{J} = \frac{1}{2m}\left[\psi^*\hat{\mathbf{p}}\psi + (\psi^*\hat{\mathbf{p}}\psi)^*\right]$$

where $\hat{\mathbf{p}}$ is the momentum operator.

7.35 Show that for a one-dimensional wavefunction of the form

$$\psi(x, t) = A \exp [i\phi(x, t)]$$

$$\mathbb{J} = \frac{\hbar}{m} |A|^2 \frac{\partial \phi}{\partial x}$$

7.36 Show that for a *wave packet* $\psi(x, t)$, one may write

$$\int_{-\infty}^{\infty} \mathbb{J}\, dx = \frac{1}{2m} (\langle p \rangle + \langle p \rangle^*) = \frac{\langle p \rangle}{m}$$

7.37 Show that a complex potential function, $V^*(x) \neq V(x)$, contradicts the continuity equation (7.97).

Lack of necessary and sufficient, incomplete description

7.38 (a) Show that if $\psi(x, t)$ is real, then

$$\mathbb{J} = 0$$

for all x.

(b) What type of wave structure does a real state function correspond to? $\psi = e^{k \cdot r}$

7.6 ONE-DIMENSIONAL BARRIER PROBLEMS

In a one-dimensional scattering experiment, the intensity and energy of the particles in the incident beam are known in addition to the structure of the potential barrier $V(x)$. Three fundamental scattering configurations are depicted in Fig. 7.17. The energy of the particles in the beam is denoted by E.

The Simple Step

Let us first consider the simple step (Fig. 7.17a) for the case $E > V$. We wish to obtain the space-dependent wavefunction φ for all x. The potential function is zero for $x < 0$ and is the constant V, for $x \geq 0$. The incident beam comes from $x = -\infty$. To construct φ we divide the x axis into two domains: region I and region II, depicted in Fig. 7.18. In region I, $V = 0$, and the time-independent Schrödinger equation appears as

$$-\frac{\hbar^2}{2m}\varphi_{xx} = E\varphi = \frac{\hbar^2 k_1^2}{2m}\varphi \tag{7.115}$$

In this domain the energy is entirely kinetic. If we set

$$\frac{\hbar^2 k_1{}^2}{2m} = E \tag{7.116}$$

then the latter equation becomes

$$\varphi_{xx} = -k_1{}^2\varphi \qquad \text{in region I} \tag{7.117}$$

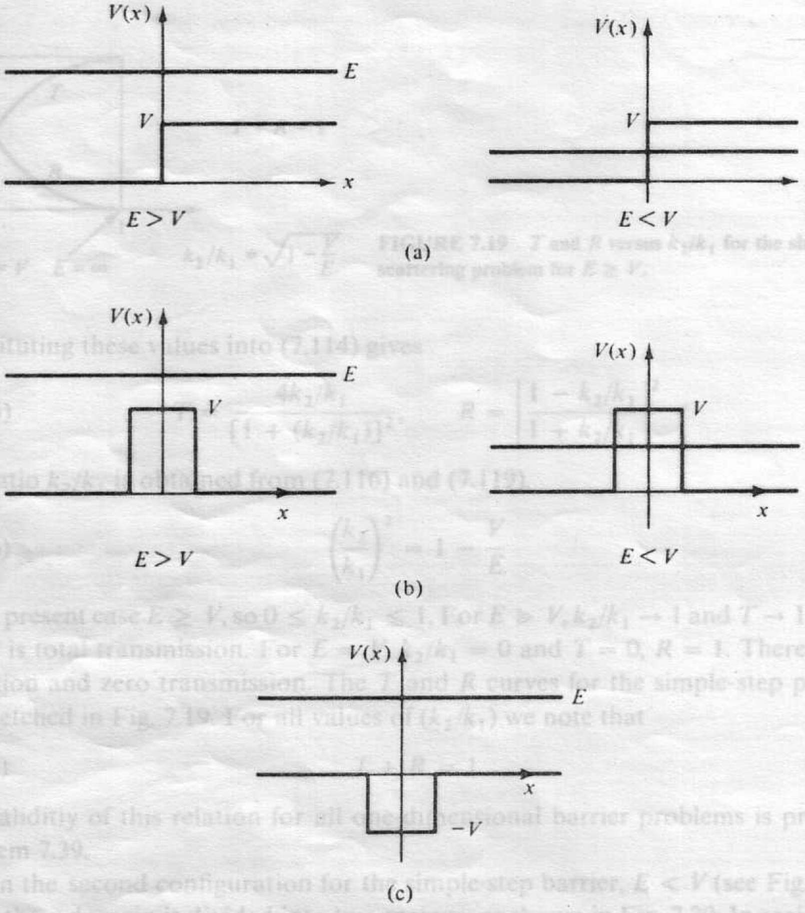


FIGURE 7.17 **(a) The simple step. (b) The rectangular barrier. (c) The rectangular well.**

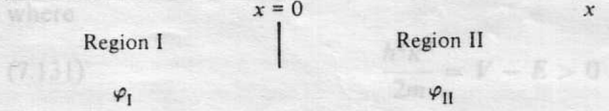


FIGURE 7.18 **Domains relevant to the simple-step scattering problem for the case $E \geq V$.**

·1 In region II the potential is the constant V and the time-independent Schrödinger equation appears as

$$-\frac{\hbar^2}{2m}\varphi_{xx} = (E - V)\varphi \tag{7.118}$$

O →

The kinetic energy decreases by V and is given by

$$\frac{\hbar^2 {k_2}^2}{2m} = E - V \tag{7.119}$$

In terms of k_2, (7.118) appears as

$$\varphi_{xx} = -{k_2}^2\varphi \qquad \text{in region II} \tag{7.120}$$

1 Writing φ_I for the solution to (7.117) and φ_II for the solution to (7.120), one obtains

$$\begin{aligned} \varphi_\text{I} &= Ae^{ik_1x} + Be^{-ik_1x} \\ \varphi_\text{II} &= Ce^{ik_2x} + De^{-ik_2x} \end{aligned} \tag{7.121}$$

Since the term De^{-ik_2x} (together with the time-dependent factor $e^{-i\omega_2 t}$) represents a wave emanating from the right ($x = +\infty$ in Fig. 7.18), and there is no such wave, we may conclude that $D = 0$. The interpretation of the remaining A, B, and C terms is given in Eq. (7.112). To repeat, $A \exp(ik_1x)$ represents the incident wave; $B \exp(-ik_1x)$, the reflected wave; and $C \exp(ik_2x)$, the transmitted wave.

2 It is important at this time to realize that φ_I and φ_II (with $D \equiv 0$) represent a single solution to the Schrödinger equation for all x, for the potential curve depicted in Fig. 7.18. Since any wavefunction and its first derivative are continuous (see Section 3.3), at the point $x = 0$ where φ_I and φ_II join it is required that

$$\begin{aligned} \varphi_\text{I}(0) &= \varphi_\text{II}(0) \\ \frac{\partial}{\partial x}\varphi_\text{I}(0) &= \frac{\partial}{\partial x}\varphi_\text{II}(0) \end{aligned} \tag{7.122}$$

3 These equalities give the relations

$$\begin{aligned} A + B &= C \\ A - B &= \frac{k_2}{k_1}C \end{aligned} \tag{7.123}$$

·2 Solving for C/A and B/A, one obtains

$$\frac{C}{A} = \frac{2}{1 + k_2/k_1}, \qquad \frac{B}{A} = \frac{1 - k_2/k_1}{1 + k_2/k_1} \tag{7.124}$$

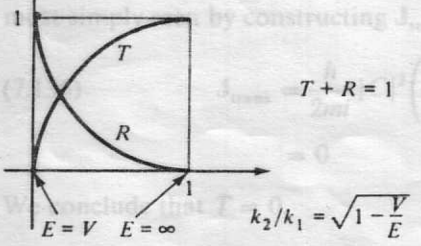


FIGURE 7.19 T **and** R **versus** k_2/k_1 **for the simple-step scattering problem for** $E \geq V$.

1 Substituting these values into (7.114) gives

$$T = \frac{4k_2/k_1}{[1 + (k_2/k_1)]^2}, \qquad R = \left|\frac{1 - k_2/k_1}{1 + k_2/k_1}\right|^2 \tag{7.125}$$

2 The ratio k_2/k_1 is obtained from (7.116) and (7.119).

$$\left(\frac{k_2}{k_1}\right)^2 = 1 - \frac{V}{E} \tag{7.126}$$

† 3 In the present case $E \geq V$, so $0 \leq k_2/k_1 \leq 1$. For $E \gg V, k_2/k_1 \to 1$ and $T \to 1, R \to 0$. There is total transmission. For $E = V$, $k_2/k_1 = 0$ and $T = 0$, $R = 1$. There is total 3' reflection and zero transmission. The T and R curves for the simple-step potential are sketched in Fig. 7.19. For all values of (k_2/k_1) we note that

$$T + R = 1 \tag{7.127}$$

The validitiy of this relation for all one-dimensional barrier problems is proved in Problem 7.39.

1' In the second configuration for the simple-step barrier, $E < V$ (see Fig. 7.17a). Again the x domain is divided into two regions, as shown in Fig. 7.20. In region I the Schrödinger equation becomes

$$\varphi_{xx} = -k_1{}^2\varphi \qquad \text{in region I} \tag{7.128}$$

where

$$\frac{\hbar^2 k_1{}^2}{2m} = E \tag{7.129}$$

1 In region II the Schrödinger equation is

$$\varphi_{xx} = \kappa^2\varphi \qquad \text{in region II} \tag{7.130}$$

where

$$\frac{\hbar^2\kappa^2}{2m} = V - E > 0 \tag{7.131}$$

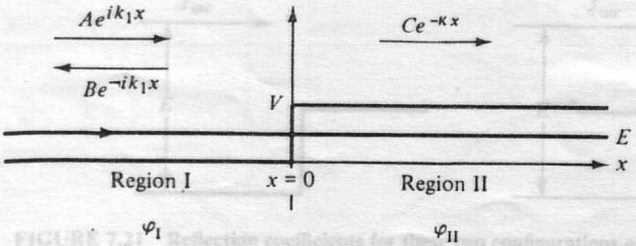


FIGURE 7.20 Domains relevant to the simple-step scattering problem for the case $E \le V$.

The kinetic energy in this domain is negative ($-\hbar^2\kappa^2/2m$). In classical physics region II is a "forbidden" domain. In quantum mechanics, however, it is possible for particles to penetrate the barrier.

3 Again calling the solution to (7.128) $\varphi_{\rm I}$ and the solution to (7.130) $\varphi_{\rm II}$, we obtain

$$\begin{aligned} \varphi_{\rm I} &= Ae^{ik_1x} + Be^{-ik_1x} \\ \varphi_{\rm II} &= Ce^{-\kappa x} \end{aligned} \tag{7.132}$$

Continuity of φ and φ_x at $x = 0$ gives

$$\begin{aligned} 1 + \frac{B}{A} &= \frac{C}{A} \\ 1 - \frac{B}{A} &= i\frac{\kappa}{k_1}\frac{C}{A} \end{aligned} \tag{7.133}$$

Solving for (C/A) and (B/A) one obtains

$$\begin{aligned} \frac{C}{A} &= \frac{2}{1 + i\kappa/k_1} \\ \frac{B}{A} &= \frac{1 - i\kappa/k_1}{1 + i\kappa/k_1} \end{aligned} \tag{7.134}$$

2 The coefficient B/A is of the form z^*/z, where z is a complex number. It follows that $|B/A| = 1$, so

$$R = \left|\frac{B}{A}\right|^2 = 1, \qquad T = 0 \tag{7.135}$$

There is total reflection, hence the transmission must be zero.

3 To obtain the latter result analytically from our equations above, we must calculate the transmitted current. The function $\varphi_{\rm II}$ is of the form of a complex amplitude times a real function of x (7.132). Such wavefunctions do not represent propagating

3· waves. They are sometimes called *evanescent waves*. That they carry no current is most simply seen by constructing $\mathbb{J}_{\text{trans}}$ (7.106).

$$\mathbb{J}_{\text{trans}} = \frac{\hbar}{2mi}|C|^2\left(e^{-\kappa x}\frac{\partial}{\partial x}e^{-\kappa x} - e^{-\kappa x}\frac{\partial}{\partial x}e^{-\kappa x}\right) \tag{7.136}$$

$$= 0$$

We conclude that $T = 0$.

PROBLEMS

7.39 Show that

$$T + R = 1$$

for all one-dimensional barrier problems.

Answer

Since the scattering process is assumed to be steady-state, the continuity equation (7.101) becomes

$$\frac{\partial \mathbb{J}_x}{\partial x} = 0$$

Integrating this equation, one obtains

$$\int_{-\infty}^{\infty}\left(\frac{\partial \mathbb{J}_x}{\partial x}\right)dx = \mathbb{J}_{+\infty} - \mathbb{J}_{-\infty} = 0$$

But

$$\mathbb{J}_{-\infty} = \mathbb{J}_{\text{inc}} - \mathbb{J}_{\text{refl}}$$

$$\mathbb{J}_{+\infty} = \mathbb{J}_{\text{trans}}$$

so that the equation above becomes

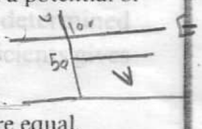
$$\mathbb{J}_{\text{trans}} + \mathbb{J}_{\text{refl}} = \mathbb{J}_{\text{inc}} \Rightarrow T + R = 1$$

Dividing through by $\mathbb{J}_{\text{inc}}$ gives the desired result.

3/ **7.40** Electrons in a beam of density $\rho = 10^{15}$ electrons/m are accelerated through a potential of 100 V. The resulting current then impinges on a potential step of height 50 V.

(a) What are the incident, reflected, and transmitted currents?

(b) Design an electrostatic configuration that gives a simple-step potential.



7.41 Show that the reflection coefficients for the two cases depicted in Fig. 7.21 are equal.

7.42 For the scattering configuration depicted in Fig. 7.20, given that $V = 2E$, at what value of x is the density in region II half the density of particles in the incident beam?

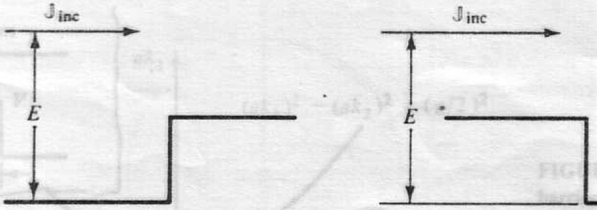


FIGURE 7.21 **Reflection coefficients for these two configurations are equal. (See Problem 7.41.)**

7.43 Equation (7.123) may be written in the matrix form

$$\begin{pmatrix} -1 & 1 \\ 1 & k_2/k_1 \end{pmatrix}\begin{pmatrix} B/A \\ C/A \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

Calling the 2 × 2 matrix $\mathscr{D}$, the left column vector $\mathscr{V}$, and the right column vector $\mathscr{U}$ permits this equation to be more simply written

$$\mathscr{D}\mathscr{V} = \mathscr{U}$$

This inhomogeneous matrix equation has the solution

$$\mathscr{V} = \mathscr{D}^{-1}\mathscr{U}$$

where $\mathscr{D}^{-1}$ is the inverse of $\mathscr{D}$, that is,

$$\mathscr{D}^{-1}\mathscr{D} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

(a) Find $\mathscr{D}^{-1}$ and then construct $\mathscr{V}$ using the technique above. Check your answer with (7.124).

(b) Do the same for (7.133) and (7.134).

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7.7 THE RECTANGULAR BARRIER. TUNNELING

The scattering configuration we now wish to examine is depicted in Fig. 7.17b. The energy of the particles in the beam is greater than the height of the potential barrier, $E > V$. For the case at hand there are three relevant domains (see Fig. 7.22):

Region I: $x < -a$, $V = 0$.
(7.137) Region II: $-a \leq x \leq +a$, $V > 0$, and constant.
Region III: $a < x$, $V = 0$.

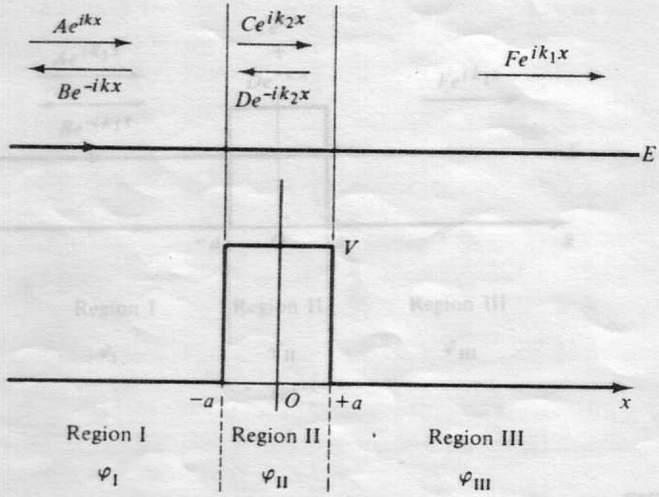

FIGURE 7.22 Domains relevant to the rectangular barrier scattering problem for the case $E \geq V$.

The solutions to the time-independent Schrödinger equation in each of the three domains are:

$$\varphi_I = Ae^{ik_1x} + Be^{-ik_1x}, \qquad \frac{\hbar^2 k_1{}^2}{2m} = E$$

$$\varphi_{II} = Ce^{ik_2x} + De^{-ik_2x}, \qquad \frac{\hbar^2 k_2{}^2}{2m} = E - V$$

$$\varphi_{III} = Fe^{ik_1x}, \qquad \frac{\hbar^2 k_1{}^2}{2m} = E \tag{7.138}$$

$$(ak_1)^2 - (ak_2)^2 = \frac{2ma^2V}{\hbar^2} \equiv \frac{g^2}{4}$$

The parameter g contains all the barrier (or well) characteristics. The latter equation (conservation of energy) reveals the simple manner in which ak_1 and ak_2 are related. In Cartesian ak_1, ak_2 space they lie on a hyperbola (Fig. 7.23). The permitted values of k_1 (and therefore E) comprise a positive unbounded continuum. For each such eigen-k_1-value, there is a corresponding eigenstate $(\varphi_I, \varphi_{II}, \varphi_{III})$ which is determined in terms of the coefficients, $(B/A, C/A, D/A, F/A)$. Knowledge of these coefficients gives the scattering parameters

$$T = \left|\frac{F}{A}\right|^2; \qquad R = \left|\frac{B}{A}\right|^2$$

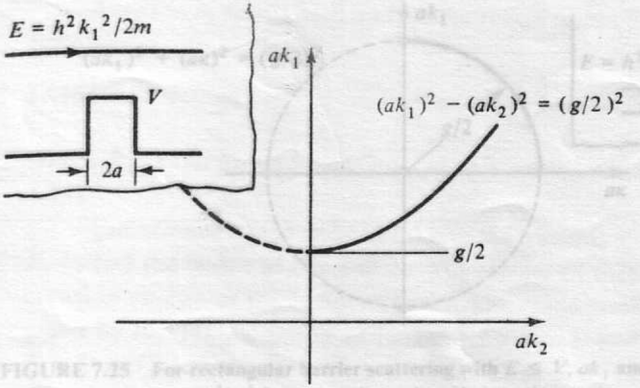

FIGURE 7.23 For rectangular-barrier scattering with $E \geq V, ak_1$ and ak_2 lie on a hyperbola.

$$ak_1 \geq ak_2 \geq 0$$

The energy spectrum $\hbar^2 k_1{}^2/2m$ comprises an unbounded continuum.

The coefficients are determined from the boundary conditions at $x = a$ and $x = -a$,

$$\begin{gathered}
e^{-ik_1 a} + \left(\frac{B}{A}\right)e^{ik_1 a} = \left(\frac{C}{A}\right)e^{-ik_2 a} + \left(\frac{D}{A}\right)e^{ik_2 a} \\
k_1\left[e^{-ik_1 a} - \left(\frac{B}{A}\right)e^{ik_1 a}\right] = k_2\left[\left(\frac{C}{A}\right)e^{-ik_2 a} - \left(\frac{D}{A}\right)e^{ik_2 a}\right] \\
\left(\frac{C}{A}\right)e^{ik_2 a} + \left(\frac{D}{A}\right)e^{-ik_2 a} = \left(\frac{F}{A}\right)e^{ik_1 a} \\
k_2\left[\left(\frac{C}{A}\right)e^{ik_2 a} - \left(\frac{D}{A}\right)e^{-ik_2 a}\right] = k_1\left(\frac{F}{A}\right)e^{ik_1 a}
\end{gathered} \tag{7.139}$$

These are four linear, algebraic, inhomogeneous equations for the four unknowns: (B/A), (C/A), (D/A), and (F/A). Solving the last two for (D/A) and (C/A) as functions of (F/A) and substituting into the first two permits one to solve for (B/A) and (F/A). These appear as

$$\begin{gathered}
\frac{F}{A} = e^{2ik_1 a}\left[\cos(2k_2 a) - \frac{i}{2}\left(\frac{k_1{}^2 + k_2{}^2}{k_1 k_2}\right)\sin(2k_2 a)\right]^{-1} \\
2\left(\frac{B}{A}\right) = i\left(\frac{F}{A}\right)\frac{k_2{}^2 - k_1{}^2}{k_1 k_2}\sin(2k_2 a)
\end{gathered} \tag{7.140}$$

The transmission coefficient is most simply obtained from the second of these, together with the relation

$$T + R = \left|\frac{F}{A}\right|^2 + \left|\frac{B}{A}\right|^2 = 1 \tag{7.141}$$

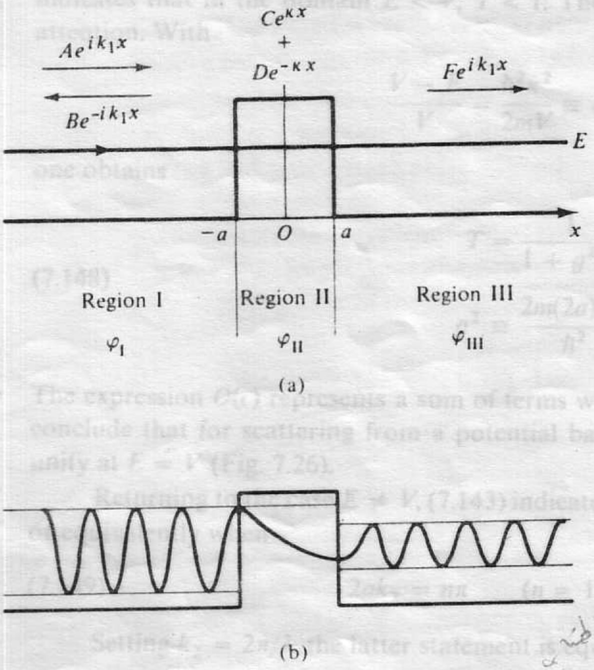

FIGURE 7.24 **(a) Domains relevant to the rectangular barrier scattering problem, for the case $E \leq V$. (b) Real part of φ for the case above, showing the hyperbolic decay in the barrier domain and decrease in amplitude of the transmitted wave.**

3 There results

$$\frac{1}{T} = \left|\frac{A}{F}\right|^2 = 1 + \frac{1}{4}\left(\frac{k_1{}^2 - k_2{}^2}{k_1 k_2}\right)^2 \sin^2(2k_2 a) \tag{7.142}$$

Rewriting k_1 and k_2 in terms of E and V as given by (7.138), one obtains

$$\boxed{\frac{1}{T} = 1 + \frac{1}{4}\frac{V^2}{E(E-V)}\sin^2(2k_2 a) \qquad E > V} \tag{7.143}$$

$\frac{\hbar^2 k_2^2}{2m} = E - V$

The reflection coefficient is $1 - T$.

1. For the case $E < V$, as depicted in Fig. 7.24a, we find that the structure of the solutions (7.138) are still appropriate, with the simple modification

$$ik_2 \to \kappa, \qquad \frac{\hbar^2\kappa^2}{2m} = V - E > 0$$
$$(ak_1)^2 + (a\kappa)^2 = \frac{2ma^2V}{\hbar^2} \equiv \frac{g^2}{4} \tag{7.144}$$

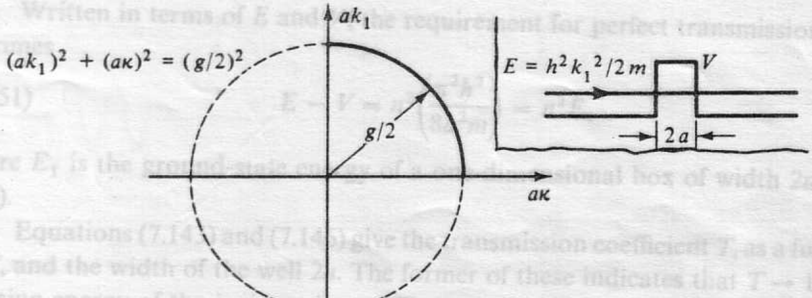

FIGURE 7.25 **For rectangular barrier scattering with $E \le V$, ak_1 and $a\kappa$ lie on a circle $ak_1 \ge 0$, $a\kappa \ge 0$. The energy spectrum $(\hbar^2 k_1{}^2/2m)$ comprises a bounded continuum.**

This latter conservation of energy statement indicates that the variables ak_1 and $a\kappa$ lie on a circle of radius $g/2$ (Fig. 7.25). The permitted eigen-k_1-values now comprise a positive, bounded continuum, so that the eigenenergies

$$E = \frac{\hbar^2 k_1{}^2}{2m}$$

also comprise a positive, bounded continuum.

The algebra leading to (7.140) remains unaltered so that the transmission coefficient for this case is obtained by making the substitution of (7.144) into (7.142). We also recall that $\sin(iz) = i \sinh z$. There results

$$\frac{1}{T} = 1 + \frac{1}{4}\left(\frac{k_1{}^2 + \kappa^2}{k_1 \kappa}\right)^2 \sinh^2(2\kappa a) \tag{7.145}$$

which, with (7.144), gives

$$\boxed{\frac{1}{T} = 1 + \frac{1}{4}\frac{V^2}{E(V-E)} \sinh^2(2\kappa a) \qquad E<V} \tag{7.146}$$

Writing this equation in terms of T,

$$\boxed{T = \frac{1}{1 + \dfrac{1}{4}\dfrac{V^2}{E(V-E)} \sinh^2(2\kappa a)} \qquad E < V} \tag{7.147}$$

2 indicates that in the domain $E < V$, $T < 1$. The limit that $E \to V$ deserves special attention. With

$$\frac{V-E}{V} = \frac{\hbar^2\kappa^2}{2mV} \equiv \epsilon \to 0$$

one obtains

$$T = \frac{1}{1 + g^2/4} + O(\epsilon)$$

$$g^2 \equiv \frac{2m(2a)^2 V}{\hbar^2} \tag{7.148}$$

The expression $O(\epsilon)$ represents a sum of terms whose value goes to zero with ϵ. We conclude that for scattering from a potential barrier, the transmission is less than unity at $E = V$ (Fig. 7.26).

Returning to the case $E \neq V$, (7.143) indicates that $T = 1$ when $\sin^2(2k_2 a) = 0$, or equivalently when

$$2ak_2 = n\pi \qquad (n = 1, 2, \ldots) \tag{7.149}$$

Setting $k_2 = 2\pi/\lambda$, the latter statement is equivalent to

$$2a = n\left(\frac{\lambda}{2}\right) \tag{7.150}$$

† 1 When the barrier width $2a$ is an integral number of half-wavelengths, $n(\lambda/2)$, the barrier becomes transparent to the incident beam; that is, $T = 1$. This is analogous to the case of total transmission of light through thin refracting layers.

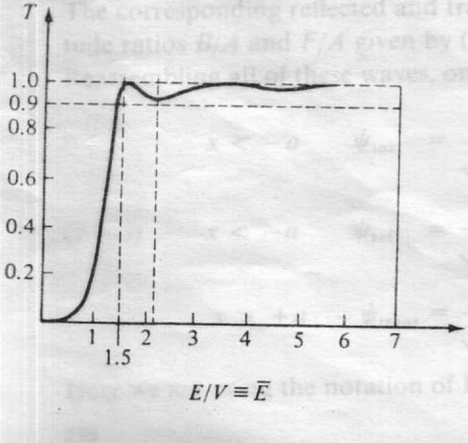

FIGURE 7.26 **Transmission coefficient T versus E/V for scattering from a rectangular barrier with $2m(2a)^2V/\hbar^2 \equiv g^2 = 16$. The additional lines are in references to Problems 7.50 et seq.**

2 Written in terms of E and V, the requirement for perfect transmission, (7.149), becomes

$$E - V = n^2\left(\frac{\pi^2\hbar^2}{8a^2m}\right) = n^2E_1 \qquad (7.151)$$

where E_1 is the ground-state energy of a one-dimensional box of width $2a$ (see Eq. 4.14).

·2 Equations (7.143) and (7.146) give the transmission coefficient T, as a function of
1 E, V, and the width of the well $2a$. The former of these indicates that $T \to 1$ with increasing energy of the incident beam. The transmission is unity for the values of E
2 given by (7.151). Equation (7.146) gives T for $E \le V$. The transmission is zero for $E = 0$ and is less than 1 for $E = V$. A sketch of T versus $E/V \equiv \bar{E}$ for the case $g^2 = 16$ is given in Fig. 7.26.

·3 The fact that T does not vanish for $E < V$ is a purely quantum mechanical
1 result. This phenomenon of particles passing through barriers higher than their own +
2 incident energy is known as *tunneling*. It allows emission of α particles from a nucleus and field emission of electrons from a metal surface in the presence of a strong electric field.

PROBLEMS

7.44 In terms of the new variables,

$$\alpha_{\pm} \equiv \frac{k_1{}^2 \pm k_2{}^2}{2k_1k_2}, \qquad \beta \equiv 2k_2a$$

$$\frac{F}{A} = \sqrt{T}\,e^{i\phi_T}, \qquad \frac{B}{A} = \sqrt{R}\,e^{i\phi_R}$$

(7.140) may be rewritten in the simpler form

$T = \left|\frac{F}{A}\right|^2 + \left|\frac{B}{A}\right|^2$

$$\frac{F}{A} = \sqrt{T}\,e^{i\phi_T} = \frac{e^{2iak_1}}{\cos\beta + i\alpha_+\sin\beta}$$

$$\left(\frac{B}{A}\right) = \sqrt{R}\,e^{i\phi_R} = i\alpha_-\sqrt{T}\,e^{i\phi_T}\sin\beta$$

Use these expressions to show:

(a) $T + R = 1$.

(b) $\phi_T = \phi_R - n(\pi/2)$, $n = 1, 2, 3, \ldots$.

(c) $\tan(\phi_T - 2k_1a) = \alpha_+ \tan\beta$

(d) What is ϕ_R for the infinite potential step: $V(x) = \infty$, $x \ge 0$; $V(x) = 0$, $x < 0$?

Answers (partial)

(a) Solving for $T + R$ from (7.140) gives

$$T + R = \frac{1 + \alpha_-{}^2\sin^2\beta}{\cos^2\beta + \alpha_+{}^2\sin^2\beta}$$

Substituting the definitions of $\alpha_{\pm}$ gives the desired result.

7.9 KINETIC PROPERTIES OF A WAVE PACKET SCATTERED FROM A POTENTIAL BARRIER

The time-dependent one-dimensional scattering problem addresses itself primarily to the problem of a wave packet incident on a potential barrier. It seeks the shape of the reflected and transmitted pulse. We will restrict our discussion to the kinematic properties of these pulses.

To formulate this problem we first construct a wave packet whose center is at $x = -X$ at $t = 0$. In previous chapters we obtained such wave packets centered at $x = 0$ at $t = 0$. They are of the form

$$\psi(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} b(k) e^{i(kx - \omega t)}\, dk \tag{7.157}$$

For this same packet to be centered at $x = -X$ initially, one merely effects a translation in x so that

$$\begin{aligned} \psi(x, t) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} b(k) e^{ik(x+X)} e^{-i\omega t}\, dk \\ &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} b(k) e^{ikX} e^{i(kx - \omega t)}\, dk \end{aligned} \tag{7.158}$$

For example, for a chopped pulse, L cm long, containing particles moving with momentum $\hbar k_0$, $b(k)$ is given by (6.32):

$$b(k) = \sqrt{\frac{2}{\pi L}} \frac{\sin (k - k_0)L/2}{k - k_0} \tag{7.159}$$

See Fig. 7.31. The group velocity of this packet is $v_0 = \hbar k_0/m$. Let us call the wave packet (7.158), ψ_{inc}. This packet is a superposition of plane-wave states of the form (7.112). Each such incident k-component plane wave is reflected and transmitted. The corresponding reflected and transmitted waves are constructed from the amplitude ratios B/A and F/A given by (7.140), which are functions of k (k_1 in Eq. 7.140). Reassembling all of these waves, one obtains

$$\begin{aligned} &x < -a \qquad \psi_{\text{inc}} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} b(k) e^{ikX} e^{i(kx - \omega t)}\, dk \\ &x < -a \qquad \psi_{\text{refl}} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \sqrt{R}\, e^{i\phi_R} b(k) e^{ikX} e^{-i(kx + \omega t)}\, dk \\ &x > +a \qquad \psi_{\text{trans}} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \sqrt{T}\, e^{i\phi_T} b(k) e^{ikX} e^{i(kx - \omega t)}\, dk \end{aligned} \tag{7.160}$$

Here we are using the notation of Problem

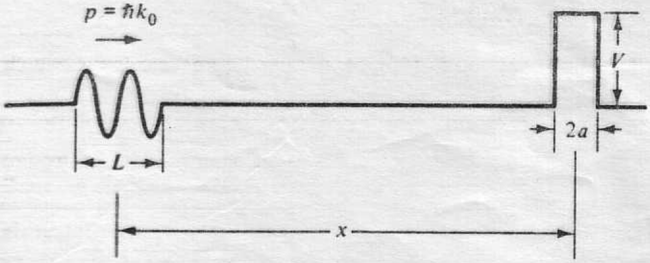

FIGURE 7.31 **Wave packet incident on a potential barrier.** $x \gg L \simeq 2a$.

To uncover the kinetic properties of these packets, we use the method of *stationary phase.* This relies on the fact that the major contribution in a Fourier integral is due to the k component with stationary phase. If we call this component k_0, then the phase of the Fourier integral for ψ_{refl} vanishes when

$$\frac{\partial}{\partial k}(\phi_R + kX - kx - \omega t) = 0 \tag{7.161}$$

This gives the trajectory of the reflected packet,

$$x = -\frac{\hbar k_0}{m}t + X + \left(\frac{\partial \phi_R}{\partial k}\right)_{k_0} \qquad x < -a \tag{7.162}$$

In like manner, for the incident and transmitted packets, one obtains

$$x = \frac{\hbar k_0}{m}t - X, \qquad x < -a \tag{7.163}$$

$$x = \frac{\hbar k_0}{m}t - X - \left(\frac{\partial \phi_T}{\partial k}\right)_{k_0}, \qquad x > a \tag{7.164}$$

The latter three equations illustrate the effect of a potential barrier on the trajectory of an incident wave packet. Were there no barrier, the packet would move freely in accordance with (7.163). However, there is a delay for both the transmitted and reflected packets. The transmitted pulse arrives at any plane $x > a$, $(\partial\phi_T/\partial k_0)v_0^{-1}$ seconds after the free pulse. The reflected pulse arrives at any plane $x < -a$, $(\partial\phi_R/\partial k_0)v_0^{-1}$ seconds after the free pulse would be reflected from an impenetrable wall at the $x = 0$ plane.[1]

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[1] The time development of a wave packet scattering from a potential barrier is graphically depicted in D. A. Saxon, *Elementary Quantum Mechanics*, Holden-Day, San Francisco, 1968.

CHAPTER 9

ANGULAR MOMENTUM

9.1 *Basic Properties*
9.2 *Eigenvalues of the Angular Momentum Operators*
9.3 *Eigenfunctions of the Orbital Angular Momentum Operators $\hat{L}^2$ and $\hat{L}_z$*
9.4 *Addition of Angular Momentum*
9.5 *Total Angular Momentum for Two or More Electrons*

1-2.3 ≡ 1. .2 3

1 *Our study of the applications of quantum mechanics to three-dimensional problems
begins with a description of the properties of angular momentum. We first consider
orbital angular momentum, which is closely akin to angular momentum encountered in*
2 *classical physics. Angular momentum in quantum mechanics, however, is a more general
concept than its classical counterpart. In quantum mechanics, in addition to orbital
angular momentum, one also encounters spin angular momentum. Spin angular momentum
is an intrinsic, or internal, property of elementary particles such as electrons and photons,*
3 *and has no classical counterpart. The operators corresponding to the Cartesian com-
ponents of angular momentum in quantum mechanics obey a set of fixed, fundamental
commutator relations. These relations are first derived for orbital angular momentum
and then employed as the defining relations for angular momentum in general. Eigen-*
4 *values of angular momentum stemming from these commutator relations are obtained,
and it is at this point that a distinction between orbital and spin angular momentum first
emerges.*

9.1 BASIC PROPERTIES

The significance of angular momentum in classical physics is that it is one of the fundamental constants of motion (together with linear momentum and energy) of an isolated system. As we will find, the counterpart of this statement also holds for isolated quantum mechanical systems. This conservation principle for angular momentum stems from the isotropy of space. That is, as described previously in Section 6.3, the physical laws relating to an isolated system are in no way dependent on the orientation of that system with respect to some fixed set of axes in space.

Classically, angular momentum of a particle is a property that depends on the particle's linear momentum **p** and its displacement **r** from some prescribed origin. It is given by (see Fig. 1.9)

$$\mathbf{L} = \mathbf{r} \times \mathbf{p} \tag{9.1}$$

One may also speak of the angular momentum of a system of particles, or of a rigid body. For such extended aggregates, one must add the angular momentum of all particles in the system to obtain the total angular momentum of the system.

Cartesian Components

The classical Cartesian components of the orbital angular momentum **L** for a particle with momentum $\mathbf{p} = (p_x, p_y, p_z)$ at the displacement $\mathbf{r} = (x, y, z)$ are

$$\begin{aligned} L_x &= yp_z - zp_y \\ L_y &= zp_x - xp_z \\ L_z &= xp_y - yp_x \end{aligned} \tag{9.2}$$

The quantum mechanical operators $\hat{L}_x$, $\hat{L}_y$, and $\hat{L}_z$, corresponding to these observables, derive their definitions directly from the classical expressions above, with $\hat{\mathbf{p}}$ replaced by its corresponding gradient operator. There follows

$$\begin{aligned} \hat{L}_x &= \hat{y}\hat{p}_z - \hat{z}\hat{p}_y = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right) \\ \hat{L}_y &= \hat{z}\hat{p}_x - \hat{x}\hat{p}_z = -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right) \\ \hat{L}_z &= \hat{x}\hat{p}_y - \hat{y}\hat{p}_x = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) \end{aligned} \tag{9.3}$$

In terms of the three-dimensional vector linear momentum operator

$$\hat{\mathbf{p}} = (\hat{p}_x, \hat{p}_y, \hat{p}_z) = -i\hbar\left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}\right) = -i\hbar\nabla \tag{9.4}$$

the equations above may be written as the single vector equation

$$\mathbf{L} = -i\hbar\mathbf{r} \times \boldsymbol{\nabla} \tag{9.5}$$

2 Commutator Relations

Let us examine the commutation properties of these operators. If, for example, $\hat{L}_x$ does not commute with $\hat{L}_y$, then these components of angular momentum cannot be simultaneously specified in a single state, that is, these operators do not have common eigenfunctions.

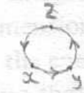
1 To examine this specific question, we employ the basic commutator relation

$$[\hat{x}, \hat{p}_x] = i\hbar \tag{9.6}$$

2 There follows

$$\begin{aligned}[\hat{L}_x, \hat{L}_y] &= \hat{L}_x\hat{L}_y - \hat{L}_y\hat{L}_x \\ &= (\hat{y}\hat{p}_z - \hat{z}\hat{p}_y)(\hat{z}\hat{p}_x - \hat{x}\hat{p}_z) - (\hat{z}\hat{p}_x - \hat{x}\hat{p}_z)(\hat{y}\hat{p}_z - \hat{z}\hat{p}_y) \quad (1) \\ &= \hat{x}\hat{p}_y(\hat{z}\hat{p}_z - \hat{p}_z\hat{z}) - \hat{y}\hat{p}_x(\hat{z}\hat{p}_z - \hat{p}_z\hat{z}) \\ &\qquad (3) \\ &= i\hbar(\hat{x}\hat{p}_y - \hat{y}\hat{p}_x) \\ &= i\hbar\hat{L}_z\end{aligned} \tag{9.7}$$

3 In similar fashion we obtain



$$\boxed{\begin{aligned}[\hat{L}_y, \hat{L}_z] &= i\hbar\hat{L}_x \\ [\hat{L}_z, \hat{L}_x] &= i\hbar\hat{L}_y \\ [\hat{L}_x, \hat{L}_y] &= i\hbar\hat{L}_z\end{aligned}} \tag{9.8}$$

These commutator relations are sometimes combined in the single vector equation

$$i\hbar\hat{\mathbf{L}} = \hat{\mathbf{L}} \times \hat{\mathbf{L}} \tag{9.9}$$

which in determinantal form appears as

$$i\hbar(\mathbf{e}_x\hat{L}_x + \mathbf{e}_y\hat{L}_y + \mathbf{e}_z\hat{L}_z) = \begin{vmatrix} \mathbf{e}_x & \mathbf{e}_y & \mathbf{e}_z \\ \hat{L}_x & \hat{L}_y & \hat{L}_z \\ \hat{L}_x & \hat{L}_y & \hat{L}_z \end{vmatrix} \tag{9.10}$$

As illustrated in Problem 9.1, only one of the three Cartesian components of angular momentum may be specified in a quantum mechanical state. Suppose, 1 for example, that φ is an eigenstate of $\hat{L}_z$. What will measurement of $\hat{L}_x$ find? To answer this question we must bring the superposition principle into play. Expand φ in the eigenstates of $\hat{L}_x$. The squares of the coefficients of expansion give the distribution of probabilities of finding different values of L_x.

Although no two values of the Cartesian components of angular momentum can be simultaneously specified in a quantum mechanical state, if one component, say the value of L_z, is specified, it is still possible to specify an additional property of angular momentum in that state. This additional property is the value of the square of the total angular momentum, L^2, or, equivalently, the magnitude of $\mathbf{L}$ $(L = \sqrt{\mathbf{L}\cdot\mathbf{L}} = \sqrt{L^2})$.

The total angular momentum operator is the vector operator

$$\hat{\mathbf{L}} = \mathbf{e}_x\hat{L}_x + \mathbf{e}_y\hat{L}_y + \mathbf{e}_z\hat{L}_z \tag{9.11}$$

from which we may form $\hat{L}^2$.

$$\hat{L}^2 = \hat{L}_x{}^2 + \hat{L}_y{}^2 + \hat{L}_z{}^2 \tag{9.12}$$

To show that there are states of a system in which L_z and L^2 are simultaneously specified, one need merely show that $\hat{L}_z$ and $\hat{L}^2$ commute. Then we know that these operators have simultaneous eigenfunctions. That is, there are states that are eigenfunctions of both $\hat{L}_z$ and $\hat{L}^2$. Let us prove the commutability of $\hat{L}_z$ and $\hat{L}^2$.

$$\begin{aligned}
[\hat{L}_z, \hat{L}^2] &= [\hat{L}_z, \hat{L}_x{}^2 + \hat{L}_y{}^2 + \hat{L}_z{}^2] \\
&= [L_z, L_x{}^2] + [L_z, L_y{}^2] + 0 \\
&= L_x[L_z, L_x] + [L_z, L_x]L_x + L_y[L_z, L_y] + [L_z, L_y]L_y \\
&= i\hbar[L_xL_y + L_yL_x - L_yL_x - L_xL_y] \\
&= 0
\end{aligned}$$

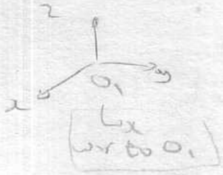
In similar manner we find that $\hat{L}_x$ and $\hat{L}_y$ also commute with $\hat{L}^2$. This must be the case because we have in no way given any special significance to the z direction. In general

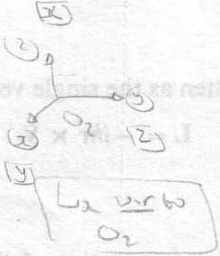
$$\begin{gathered}
[\hat{L}_x, \hat{L}^2] = [\hat{L}_y, \hat{L}^2] = [\hat{L}_z, \hat{L}^2] = 0 \\
[\hat{\mathbf{L}}, \hat{L}^2] = 0
\end{gathered} \tag{9.13}$$

It follows that the Cartesian components of $\hat{\mathbf{L}}$ have simultaneous eigenfunctions with $\hat{L}^2$. However, the individual components of $\hat{\mathbf{L}}$ do not have common eigenstates with one another (except for the special case of zero angular momentum). These properties are depicted in a Venn diagram in Fig. 9.1.

The preceding discussion tells us that $\hat{L}^2$ and $\hat{L}_z$, say, have common eigenfunctions. Let us call these eigenfunctions φ_{lm}. The integral indices l and m are related to the eigenvalues of $\hat{L}^2$ and $\hat{L}_z$ as in the following eigenfunction equations.

$$\begin{aligned}
\hat{L}^2\varphi_{lm} &= \hbar^2 l(l+1)\varphi_{lm} \qquad && (l = 0, 1, 2, \ldots) \\
\hat{L}_z\varphi_{lm} &= \hbar m\varphi_{lm} && (m = -l, \ldots, +l \text{ in integral steps})
\end{aligned} \tag{9.14}$$





w.r to O_1, O_2 has measured L_z,

and it seems that w.r to the system L both measured L_x

1st let O_1 measures L_{x_1} and then Let O_2 measures L_{x_2}

each w.r to his own state to both observe the same eigenstate. ??

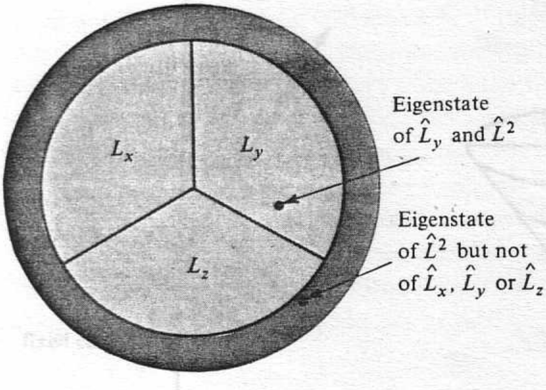

L_x
L_y
L_z
Eigenstate of $\hat{L}_y$ and $\hat{L}^2$
Eigenstate of $\hat{L}^2$ but not of $\hat{L}_x$, $\hat{L}_y$ or $\hat{L}_z$

FIGURE 9.1 Venn diagram for the eigenstates of $\hat{L}_x$, $\hat{L}_y$, $\hat{L}_z$, and $\hat{L}^2$. Every point represents an eigenfunction of $\hat{L}^2$. Depending on which sector the point is in, it is also an eigenfunction of $\hat{L}_x$, $\hat{L}_y$, or $\hat{L}_z$. The state at the center is the null eigenvector of $\hat{\mathbf{L}}$ and $\hat{L}^2$. It corresponds to the eigenvalues $L_x = L_y = L_z = 0$. Peripheral points depict states that are eigenstates of $\hat{L}^2$ only. Can you think of one such function? Note that the space of eigenstates of $\hat{L}^2$ is "bigger" than the space containing all the eigenstates of $\hat{L}_x$, $\hat{L}_y$, and $\hat{L}_z$. Compare with Fig. 5.12.

1 (These equations are derived in the next section.) The form of the first equation
indicates the following. Suppose that a system (e.g., a wheel) is rotating somewhere
in space, far removed from other objects. We measure the magnitude of its angular
2 momentum. What possible values can be found? The values that experiment finds
are only of the form $L = \hbar\sqrt{l(l+1)}$, where l is some integer. For example, one
would never measure the value $L = \hbar\sqrt{7}$, since it is not of the form $L^2 = \hbar^2 l(l+1)$.
There is no integer for which $l(l+1) = 7$. This is similar to the fact that a particle
in a one-dimensional box is never found to have the energy $E = 7E_1$. This value
does not fit the energy eigenvalue recipe $E = n^2 E_1$.

3 Suppose that we measure the magnitude of angular momentum of the wheel and find the value $L^2 = 30\hbar^2$. This corresponds to the l value $l = 5$. Having measured L^2, the system is left in an eigenstate of $\hat{L}^2$. What value does subsequent measurement of L_z yield? The answer is given by the form of the eigenvalues of $\hat{L}_z$ given in (9.14). For the case in point, since $l = 5$, L_z can *only* be found to have one of the eleven values

$$L_z = 5\hbar, 4\hbar, 3\hbar, 2\hbar, \hbar, 0, -\hbar, -2\hbar, -3\hbar, -4\hbar, -5\hbar$$

Suppose that measurement finds $L_z = 3\hbar$. Then the wheel is left in the state $\varphi_{5,3}$.

3· The form of equations (9.14) indicates that the eigenvalues of $\hat{L}^2$ are $(2l+1)$-fold degenerate. For the problem considered, all the eleven states $\varphi_{5,5}; \varphi_{5,4}; \cdots; \varphi_{5,-5}$ correspond to the same value of L^2 (i.e., $L^2 = 30\hbar^2$). (See Fig. 9.2.)

3· Uncertainty Relations

Angular momentum is a vector. The magnitude of this vector is given by L^2. Having measured L^2, is it possible to measure any of the three Cartesian components of **L**

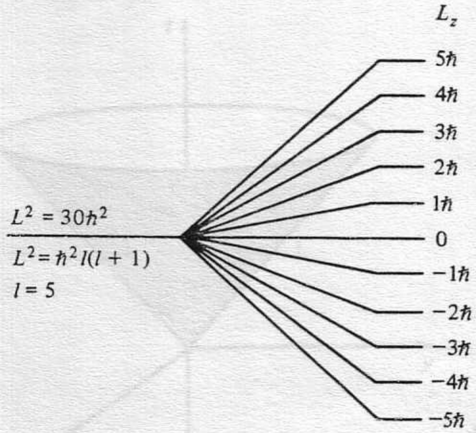


FIGURE 9.2 **The eigenvalue $L^2 = \hbar^2 l(l+1)$ is $(2l+1)$-fold degenerate. For a fixed magnitude, $L = \hbar\sqrt{l(l+1)}$, there are only $2l+1$ possible projections of L onto a given axis. (See Fig. 9.3c.)**

and leave the system (such as a wheel, a particle, an atom, a rigid rod, etc.) with the same value of L^2 that it had before measurement? Specifically, suppose that we measure L^2 and L_z and find the values $56\hbar^2$ and $3\hbar$, respectively ($l = 7$, $m = 3$). We know that the system is left in a simultaneous eigenstate of L^2 and L_z, namely, $\varphi_{7,3}$.

-1

1 It is impossible to further resolve the state of the system. We cannot obtain
the Same more information on the vector **L** without destroying part of the information already
For
George 2 known. Suppose that L_x is measured and the value $5\hbar$ is found. In measuring L_x, the information about L_z previously determined is destroyed.[1] The system is left
3 in a simultaneous eigenstate of $\hat{L}^2$ and $\hat{L}_x$. Since this is not an eigenstate of $\hat{L}_z$, subsequent measurement of L_z is not certain to yield any specific value. Similarly for measurement of L_y. This conclusion is contained in the uncertainty relation

$$\Delta L_y \, \Delta L_z \geq \frac{\hbar}{2} |\langle L_x \rangle| = \frac{\hbar L_x}{2} = \frac{5\hbar^2}{2} \tag{9.15}$$

-2

Consider the case of a wheel whose center is fixed in space. L^2 and L_z are
1 measured. What motion of the wheel will preserve these values but not preserve L_x and L_y? A very worthwhile model for such motion is given by a classical solution in which the angular momentum vector of constant magnitude precesses about the z axis at a constant inclination to that axis (see Fig. 9.3), thereby maintaining L_z. (Such motion is realized by a spinning top, with fixed vertex, in a gravity field.)

-3 In the classical problem **L** is precisely determined as a function of time. At any instant **L** may be observed and completely specified. Not so for the quantum
1 mechanical motion. If the wheel is in an eigenstate of $\hat{L}^2$ and $\hat{L}_z$, it is in a superposition

---

[1] That is, the outcome of subsequent measurement of L_z is rendered more uncertain.

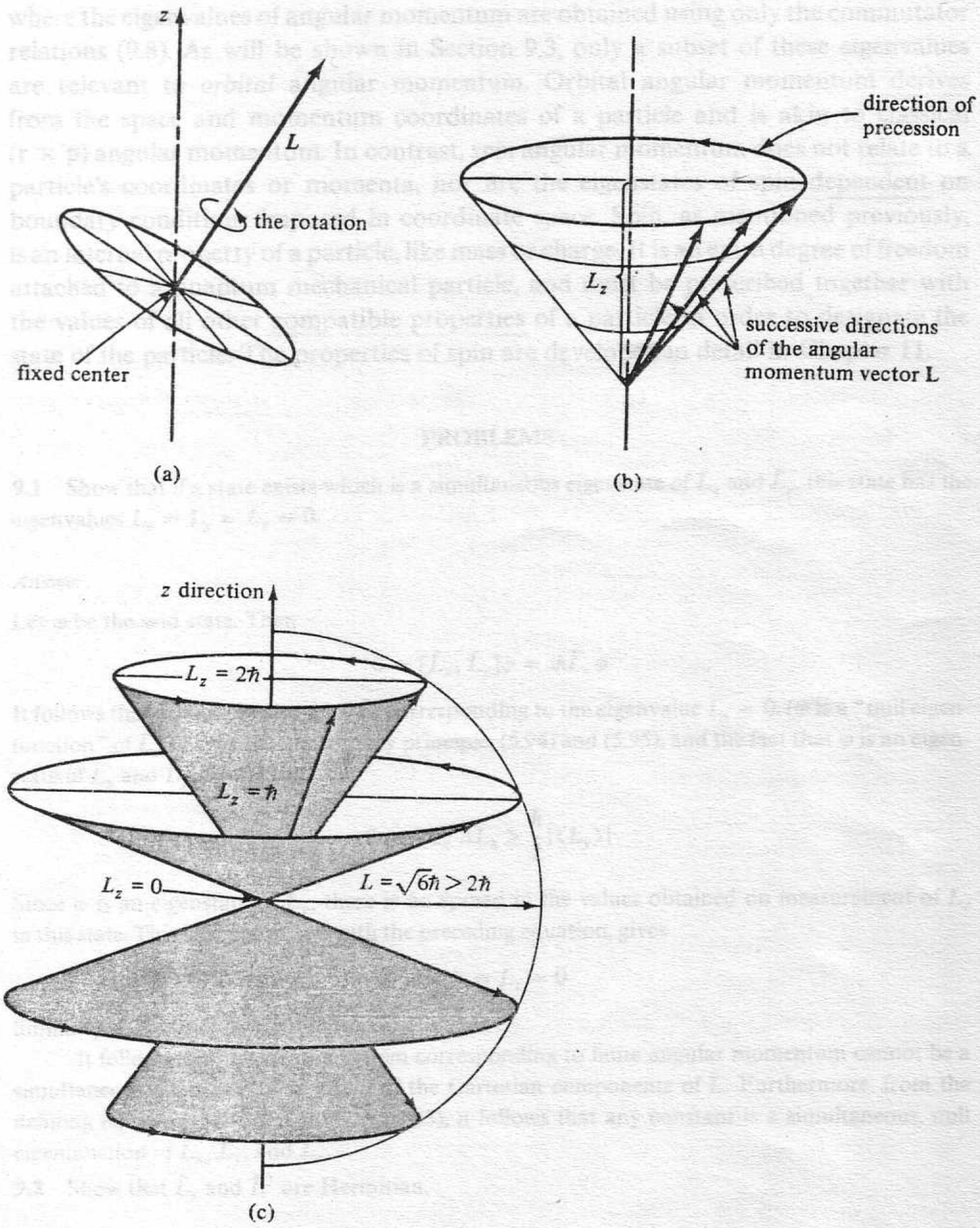


FIGURE 9.3 **(a) The angular momentum vector L of a rotating wheel whose center is fixed in space. (b) Classical precession of L about the z axis with the constant projection L_z. (c) For $l = 2$, $L^2 = 6\hbar^2$. The only possible orientations of L onto the z axis are the five values shown. The precessional motion depicted preserves L^2 and L_z. $\theta = \cos^{-1} 2/\sqrt{6}$ is the smallest possible angle between L and the z axis.**

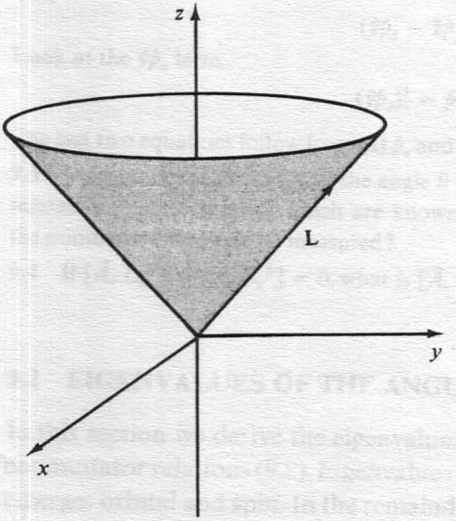


FIGURE 9.4 **For the quantum mechanical state in which L^2 and L_z are specified, L may be pictured as being uniformly distributed over the surface of a cone with half-apex-angle $\theta = \cos^{-1} m/\sqrt{l(l+1)}$.**

state (i.e., a linear combination of the eigenstates) of $\hat{L}_x$ or $\hat{L}_y$. At best one can only
2 speak of the *probability* of finding a certain value of L_x or L_y. If a system is in such
a state with definite l and m values, it is therefore more consistent to view the related
configuration as one in which the **L** vector is uniformly spread over a cone about the
z axis with half apex angle $\theta = \cos^{-1} m/\sqrt{l(l+1)}$ (see Fig. 9.4).

-4 For a given value of L [i.e., $\hbar\sqrt{l(l+1)}$] the maximum value of L_z is $\hbar l$. But
$l < \sqrt{l(l+1)}$. It follows that the angular momentum vector is never aligned with
1 a given axis. Furthermore, there are only a discrete, finite $(2l+1)$ number of in-
clinations that **L** makes with any given axis. This extraordinary property (classical
2 physics permits a continuum of inclinations) is sometimes called the *quantization
of space*. For reasons that will become clear in the following sections, l is often
referred to as the *orbital quantum number* while m is often referred to as the *azimuthal*
or *magnetic quantum number*.

4

Orbital Versus Spin Angular Momentum

The commutator relations (9.8) are the trademark of angular momentum in quantum
mechanics. Although they are consistent with the differential and coordinate-
momentum operator relations (9.3 et seq.), they may be taken independent of these
and assumed to be the defining relations for quantum mechanical angular momentum.
-1 + When such is the case, angular momentum need not refer to the space coordinates
or linear momentum components of a particle, since the relations (9.8) by them-
1 selves do not. The first example that incorporates this concept is given in Section 9.2,

where the eigenvalues of angular momentum are obtained using only the commutator
2 relations (9.8). As will be shown in Section 9.3, only a subset of these eigenvalues
are relevant to *orbital* angular momentum. Orbital angular momentum derives
from the space and momentum coordinates of a particle and is akin to classical
.2 (**r** × **p**) angular momentum. In contrast, *spin* angular momentum does not relate to a
particle's coordinates or momenta, nor are the eigenstates of spin dependent on
boundary conditions imposed in coordinate space. Spin, as mentioned previously,
1 is an internal property of a particle, like mass or charge. It is an extra degree of freedom
2 attached to a quantum mechanical particle, and must be prescribed together with
the values of all other compatible properties of a particle in order to designate the
state of the particle. The properties of spin are developed in detail in Chapter 11.

(no insight) rigorize

PROBLEMS

9.1 Show that if a state exists which is a simultaneous eigenstate of $\hat{L}_x$ and $\hat{L}_y$, this state has the eigenvalues $L_x = L_y = L_z = 0$.

Answer

Let φ be the said state. Then

$$0 = [\hat{L}_x, \hat{L}_y]\varphi = i\hbar\hat{L}_z\varphi$$

It follows that φ is an eigenstate of $\hat{L}_z$ corresponding to the eigenvalue $L_z = 0$. (φ is a "null eigenfunction" of $\hat{L}_z$.) From the uncertainty principle, (5.94) and (5.95), and the fact that φ is an eigenstate of $\hat{L}_x$ and $\hat{L}_y$ we find that

$$0 = \Delta L_x \, \Delta L_z \geq \frac{\hbar}{2}|\langle L_y\rangle|$$

Since φ is an eigenstate of $\hat{L}_y$, there is no spread in the values obtained on measurement of L_y in this state. This fact, combined with the preceding equation, gives

$$\langle L_y\rangle = L_y = 0$$

Similarly, $L_x = 0$.

It follows that a state of a system corresponding to finite angular momentum cannot be a simultaneous eigenstate of any two of the Cartesian components of $\hat{\mathbf{L}}$. Furthermore, from the defining equations for $\hat{L}_x$, $\hat{L}_y$, and $\hat{L}_z$ (9.3), it follows that any constant is a simultaneous, null eigenfunction of $\hat{L}_x$, $\hat{L}_y$, and $\hat{L}_z$.

9.2 Show that $\hat{L}_x$ and $\hat{L}^2$ are Hermitian.

Answer (partial)

To prove the Hermiticity of $\hat{L}_x$, we must show that

$$\hat{L}_x = \hat{L}_x{}^\dagger$$

or, equivalently, that

$$(\hat{y}\hat{p}_z - \hat{z}\hat{p}_y)^\dagger = (\hat{y}\hat{p}_z - \hat{z}\hat{p}_y)$$

Look at the $\hat{y}\hat{p}_z$ term.

$$(\hat{y}\hat{p}_z)^\dagger = \hat{p}_z{}^\dagger\hat{y}^\dagger = \hat{p}_z\hat{y} = \hat{y}\hat{p}_z$$

The last two equalities follow from (a) $\hat{p}_z$ and $\hat{y}$ are Hermitian, and (b) $[\hat{y}, \hat{p}_z] = 0$.

9.3 Measurements are made of the angle θ that $\mathbf{L}$ makes with the x axis of a collection of noninteracting rotators, all of which are known to have angular momentum $L = \hbar\sqrt{56}$. What is the minimum θ that will be measured?

$\text{Cos}^{-1}(\sqrt{7/8})$

9.4 If $[\hat{A}, \hat{L}_x{}^2] = [\hat{A}, \hat{L}_y{}^2] = 0$, what is $[\hat{A}, \hat{L}^2]$?

9.2 EIGENVALUES OF THE ANGULAR MOMENTUM OPERATORS

In this section we derive the eigenvalues of angular momentum that follow from the commutator relations (9.8). Eigenvalues relevant to two classes of angular momentum emerge: orbital and spin. In the remainder of the text $\hat{\mathbf{J}}$ will be used to denote angular momentum in general while $\hat{\mathbf{L}}$ will be reserved for orbital angular momentum and $\hat{\mathbf{S}}$ for spin. The operator $\hat{\mathbf{J}}$ may represent $\hat{\mathbf{L}}$, or $\hat{\mathbf{S}}$, or the combination $\hat{\mathbf{L}} + \hat{\mathbf{S}}$. The defining relations for the components of $\hat{\mathbf{J}}$ are:

$$\begin{aligned} [\hat{J}_x, \hat{J}_y] &= i\hbar\hat{J}_z \\ [\hat{J}_y, \hat{J}_z] &= i\hbar\hat{J}_x \\ [\hat{J}_z, \hat{J}_x] &= i\hbar\hat{J}_y \end{aligned} \tag{9.16}$$

$$\hat{J}^2 = \hat{J}_x{}^2 + \hat{J}_y{}^2 + \hat{J}_z{}^2 \tag{9.17}$$

The components of $\hat{\mathbf{J}}$ obey all rules obtained above from the commutator relations (9.8). These include:

$$\begin{gathered} [\hat{J}_x, \hat{J}^2] = [\hat{J}_y, \hat{J}^2] = [\hat{J}_z, \hat{J}^2] = 0 \\ \Delta J_x\,\Delta J_y \geq \frac{\hbar}{2}\,|\langle J_z\rangle| \end{gathered} \tag{9.18}$$

Ladder Operators

We seek the eigenvalues of $\hat{J}^2$ and $\hat{J}_z$. To facilitate the derivation we introduce the "ladder operators" $\hat{J}_+$ and $\hat{J}_-$. The reader will find these similar to the annihilation and creation operators $(\hat{a}, \hat{a}^\dagger)$ introduced in Section 7.2. The ladder operators are defined according to

$$\begin{aligned} \hat{J}_+ &= \hat{J}_x + i\hat{J}_y \\ \hat{J}_- &= \hat{J}_x - i\hat{J}_y = \hat{J}_+{}^\dagger \end{aligned} \tag{9.19}$$

·2 Some immediate properties of these operators are

$$
\begin{aligned}
&[\hat{J}_z, \hat{J}_+] = \hbar\hat{J}_+ \\
&[\hat{J}_z, \hat{J}_-] = -\hbar\hat{J}_-
\end{aligned}
\qquad \boxed{[\hat{J}_z, \hat{J}_\pm] = \pm\hbar\hat{J}_\pm}
$$

(9.20)

$$
\begin{aligned}
&[\hat{J}^2, \hat{J}_+] = 0 \\
&[\hat{J}^2, \hat{J}_-] = 0
\end{aligned}
\qquad \boxed{[\hat{J}^2, \hat{J}_\pm] = 0}
$$

The latter two equations follow from (9.8). To establish the first two relations one merely inserts the definitions of $\hat{J}_+$ and $\hat{J}_-$. For example,

$$
\begin{aligned}
(9.21)\qquad [\hat{J}_z, \hat{J}_+] &= [\hat{J}_z, \hat{J}_x + i\hat{J}_y] = [\hat{J}_z, \hat{J}_x] + i[\hat{J}_z, \hat{J}_y] \\
&= i\hbar\hat{J}_y - i\cdot i\hbar\hat{J}_x = \hbar(\hat{J}_x + i\hat{J}_y) = \hbar\hat{J}_+
\end{aligned}
$$

Other relations that $\hat{J}_+$ and $\hat{J}_-$ satisfy are

$$
\begin{aligned}
\hat{J}^2 &= \hat{J}_-\hat{J}_+ + \hat{J}_z{}^2 + \hbar\hat{J}_z \\
&= \hat{J}_+\hat{J}_- + \hat{J}_z{}^2 - \hbar\hat{J}_z
\end{aligned}
\qquad \boxed{\hat{J}^2 = \hat{J}_\mp\hat{J}_\pm + \hat{J}_z{}^2 \pm \hbar\hat{J}_z}
$$

(9.22)

$$[\hat{J}_+, \hat{J}_-] = 2\hbar J_z$$

Consider the relation

$$
\begin{aligned}
(9.23)\qquad \hat{J}^2 &= (\hat{J}_x - i\hat{J}_y)(\hat{J}_x + i\hat{J}_y) + \hat{J}_z{}^2 + \hbar\hat{J}_z \\
&= \hat{J}_x{}^2 + \hat{J}_y{}^2 + \hat{J}_z{}^2 + i(\hat{J}_x\hat{J}_y - \hat{J}_y\hat{J}_x) + \hbar\hat{J}_z
\end{aligned}
$$

·3 With these relations between $\hat{J}^2$, $\hat{J}_z$, $\hat{J}_+$, and $\hat{J}_-$ established we turn to construction of the eigenvalues of $\hat{L}_z$ and $\hat{L}^2$.

Let

$$(9.24)\qquad \hat{J}_z\varphi_m = \hbar m\varphi_m$$

1 We wish to show that m is either an integer or an odd multiple of one-half. Consider the operation

$$
\begin{aligned}
(9.25)\qquad \hat{J}_z\hat{J}_+\varphi_m &= (\hbar\hat{J}_+ + \hat{J}_+\hat{J}_z)\varphi_m = (\hbar\hat{J}_+ + \hat{J}_+\hbar m)\varphi_m \\
\hat{J}_z(\hat{J}_+\varphi_m) &= \hbar(m+1)(\hat{J}_+\varphi_m)
\end{aligned}
$$

where we have employed (9.21). The latter equation (9.25) implies that $\hat{J}_+\varphi_m$ is an (unnormalized) eigenfunction of $\hat{J}_z$ corresponding to the eigenvalue $\hbar(m+1)$. That is,

$$(9.26)\qquad \hat{J}_+\varphi_m = \varphi_{m+1}$$

2 Applying $\hat{J}_+$ again gives

$$(9.27)\qquad \hat{J}_+(\hat{J}_+\varphi_m) = \hat{J}_+\varphi_{m+1} = \varphi_{m+2}$$

In a similar manner, we obtain

$$\hat{J}_{-}\varphi_m = \varphi_{m-1}, \qquad \hat{J}_{-}\varphi_{m-1} = \varphi_{m-2} \tag{9.28}$$

Thus we have found a scheme of generating a sequence of (unnormalized) eigenfunctions of $\hat{J}_z$ from a single eigenfunction φ_m, with successive values of m in the sequence differing by unity.

$$(\ldots, \varphi_{m-2}, \varphi_{m-1}, \varphi_m, \varphi_{m+1}, \varphi_{m+2}, \ldots) \tag{9.29}$$

Since $\hat{J}^2$ commutes with $\hat{J}_z$, these operators have common eigenfunctions. Let φ_m be a common eigenfunction with the eigenvalue $\hbar^2 K^2$, that is,

$$\hat{J}^2\varphi_m = \hbar^2 K^2 \varphi_m \tag{9.30}$$

Operating on this equation with $\hat{J}_+$ gives [using the third equation in (9.20)]

$$\hat{J}_+\hat{J}^2\varphi_m = \hbar^2K^2(\hat{J}_+\varphi_m) = \hat{J}^2(\hat{J}_+\varphi_m) \tag{9.31}$$

The last equality asserts that $\hat{J}_+\varphi_m = \varphi_{m+1}$ is also an eigenfunction of $\hat{J}^2$ corresponding to the eigenvalue $\hbar^2K^2$. It follows that the sequence of eigenfunctions of $\hat{J}_z$ found previously (9.29) are all eigenfunctions of $\hat{J}^2$ corresponding to the same eigenvalue $\hbar^2K^2$. How many such eigenfunctions are there? From (9.30) one obtains

$$\begin{aligned} \langle J^2\rangle = \hbar^2K^2 &= \langle J_x{}^2\rangle + \langle J_y{}^2\rangle + \langle J_z{}^2\rangle \\ \hbar^2K^2 &= \langle J_x{}^2\rangle + \langle J_y{}^2\rangle + \hbar^2m^2 \end{aligned} \tag{9.32}$$

where the average has been taken in the φ_m state. It follows that

$$\hbar^2K^2 \geq \hbar^2m^2 \tag{9.33}$$

(recall $\langle J_x{}^2\rangle \geq 0$; see Problem 4.13) or, equivalently,

$$|K| \geq |m| \tag{9.34}$$

For a given value of $K > 0$, the possible values of m in the sequence (9.29) fall between $+K$ and $-K$. If $m_{\max}$ is the maximum value that m can assume for a given magnitude of angular momentum, $\hbar K$, then

$$\hat{J}_+\varphi_{m_{\max}} = 0 \tag{9.35}$$

Similarly,

$$\hat{J}_-\varphi_{m_{\min}} = 0 \tag{9.36}$$

From (9.22) and the last two equations, one obtains

$$\begin{aligned} \hat{J}^2\varphi_{m_{\max}} &= \hbar^2K^2\varphi_{m_{\max}} = \hat{J}_z{}^2\varphi_{m_{\max}} + \hbar\hat{J}_z\varphi_{m_{\max}} \\ \hbar^2K^2 &= \hbar^2m_{\max}(m_{\max}+1) \\ \hat{J}^2\varphi_{m_{\min}} &= \hbar^2K^2\varphi_{m_{\min}} = \hat{J}_z{}^2\varphi_{m_{\min}} - \hbar\hat{J}_z\varphi_{m_{\min}} \\ \hbar^2K^2 &= \hbar^2m_{\min}(m_{\min}-1) \end{aligned} \tag{9.37}$$

1 $\hat{J}^2 = \hat{J}^2_{\boxed{-}} J_+ + \hat{J}_z^2 \boxed{+} \hbar \hat{J}_z$, If we start with φ_{max} →

we must use $\hat{J}_+$ with it → $\hat{J}^2 = \hat{J}_- \hat{J}_+ + \hat{J}_z^2 + \hbar \hat{J}_z$

$$\hat{J}^2 \varphi_{max} = \underline{\hat{J}_- \hat{J}_+ \varphi_{max}} + \hat{J}_z^2 \varphi_{max} + \hbar \hat{J}_z \varphi_{max} =$$

$$\hat{J}_-(0) + (\quad \underline{z} \quad) \qquad (9.37)$$

2 When we start with φ_{min} → we must use $\hat{J}^2 = \hat{J}_{\textcircled{+}} \hat{J}_- + \hat{J}_z^2 \textcircled{-} \hbar \hat{J}_z$

3 The purpose for 1 and 2 above, is that we want a relation between K and $m_{max.}$ and $m_{min.}$, and this $\hat{J}^2 \varphi_{\substack{min. \\ max.}}$ lead to equality.

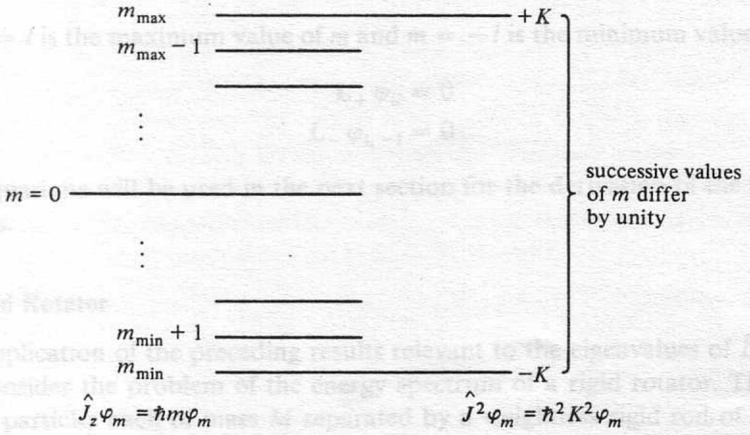

$m_{\max}$
$m_{\max} - 1$
$+K$
$m = 0$
successive values of m differ by unity
$m_{\min} + 1$
$m_{\min}$
$-K$
$\hat{J}_z \varphi_m = \hbar m \varphi_m$
$\hat{J}^2 \varphi_m = \hbar^2 K^2 \varphi_m$

FIGURE 9.5 The possible values that m may assume, for a given value of $J^2 = \hbar^2 K^2$, form a symmetric sequence about $m = 0$.

It follows that

(9.38)
$$m_{\max}(m_{\max} + 1) = m_{\min}(m_{\min} - 1)$$

which is satisfied if

(9.39)
$$m_{\max} = -m_{\min}$$

The possible values that m may assume for a given value of J^2 form a symmetric sequence about $m = 0$ (see Fig. 9.5).

Let us call

(9.40)
$$m_{\max} \equiv j$$

Since m runs from $-j$ to $+j$ in unit steps, one obtains

(9.41)
$$\begin{array}{ll} j = \text{an integer} & \text{if } m = 0 \text{ is included in the sequence of } m \text{ values} \\ j = \tfrac{1}{2} \times \text{an odd integer} & \text{if } m = 0 \text{ is not included in the sequence of } m \text{ values} \end{array}$$

Furthermore, if j is an integer, the related m values are integers. If j is an odd multiple of one-half, the related m values are odd multiples of one-half (Fig. 9.6).

In either case, inserting $j = m_{\max} = -m_{\min}$ into (9.37) gives the form of the eigenvalues of $\hat{J}^2$.

(9.42)
$$J^2 = \hbar^2 K^2 = \hbar^2 j(j + 1)$$

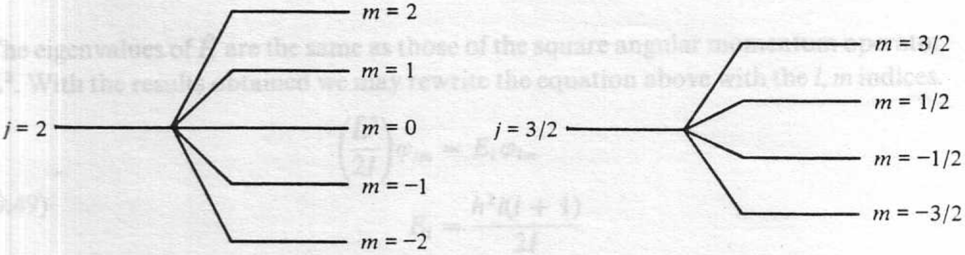


FIGURE 9.6 The angular momentum quantum number j, which enters in the eigenvalue expression $J^2 = \hbar^2 j(j+1)$, may be either integral or an odd multiple of one-half. In either case, for a given value of j, the azimuthal quantum number, m, runs from $-j$ to $+j$ in unit steps.

Angular Momentum Eigenstates

In this manner we find that the eigenvalues of $\hat{J}^2$ and $\hat{J}_z$ take the form

$$\begin{aligned} J^2 &= \hbar^2 j(j+1) \\ J_z &= \hbar m_j \qquad (m_j = -j, \ldots, +j) \end{aligned} \tag{9.43}$$

with j an integer or half an odd integer. The structure of these eigenvalue equations is very significant and is another trademark of quantum mechanical angular momentum. In that they stem directly from the commutation relations (9.16), which in turn are obeyed by all quantum mechanical angular momenta, it follows that such eigenvalue relations are also appropriate to orbital angular momentum, $\hat{\mathbf{L}}$; spin angular momentum, $\hat{\mathbf{S}}$; or their sum, $\hat{\mathbf{L}} + \hat{\mathbf{S}}$. Such, for example, are the eigenvalues of $\hat{L}^2$, $\hat{L}_z$ as given in (9.14).

As will be shown in the following section, boundary conditions imposed on the common eigenstates of $\hat{L}^2$, $\hat{L}_z$ infer that the related eigenvalues (l, m_l) be integral. Thus, of the entire spectrum of quantum angular momentum j values, only a subset ($l = j =$ integer) correspond to orbital angular momentum. The complete j spectrum (integral and half-odd-integral values) will be found to correspond to either spin angular momentum or the combination of spin plus orbital angular momentum. An example of the latter case is given by atomic electrons which have both orbital and spin angular momentum and for which one must write $\hat{\mathbf{J}} = \hat{\mathbf{L}} + \hat{\mathbf{S}}$. For the present we will concentrate on orbital angular momentum.

The eigenvalue equations for the orbital angular momentum operators $\hat{L}^2$ and $\hat{L}_z$ (with m written for m_l), together with the equations for $\hat{L}_\pm$, appear as

$$\begin{aligned} \hat{L}^2 \varphi_{lm} &= \hbar^2 l(l+1) \varphi_{lm} \\ \hat{L}_z \varphi_{lm} &= \hbar m \varphi_{lm} \qquad (m = -l, \ldots, +l) \\ \hat{L}_+ \varphi_{lm} &= \varphi_{l, m+1} \qquad (\hat{L}_+ = \hat{L}_x + i\hat{L}_y) \\ \hat{L}_- \varphi_{lm} &= \varphi_{l, m-1} \qquad (\hat{L}_- = \hat{L}_x - i\hat{L}_y) \end{aligned} \tag{9.44}$$

Since $m = l$ is the maximum value of m and $m = -l$ is the minimum value of m,

$$L_+ \varphi_{ll} = 0 \qquad (9.45)$$
$$L_- \varphi_{l,-l} = 0$$

These equations will be used in the next section for the derivation of the φ_{lm} eigenfunctions.

3. The Rigid Rotator

As an application of the preceding results relevant to the eigenvalues of $\hat{L}^2$ and $\hat{L}_z$, let us consider the problem of the energy spectrum of a rigid rotator. The rotator has two particles each of mass M separated by a weightless rigid rod of length $2a$.
! The midpoint of the rotator is fixed in space (Fig. 9.7). The moment of inertia of the rotator, taken about this point, is

$$I = 2Ma^2$$

2 Let the rotator be far removed from any force fields so that its energy is purely kinetic.

$E = \frac{1}{2} m v^2 = \frac{1}{2} m (r\dot{\theta})^2 = \frac{1}{2} m r^2 \dot{\theta}^2$,

$L = r(m r \dot{\theta})$, $L^2 = m^2 r^4 \dot{\theta}^2 \Rightarrow$

$E = \frac{1}{2} \frac{m^2}{m} \frac{r^2}{r^2} r^2 \dot{\theta}^2 = \frac{L^2}{2I}$

$$E = \frac{L^2}{2I} \qquad (9.46)$$

The quantum mechanical Hamiltonian operator is

$$\hat{H} = \frac{\hat{L}^2}{2I} \qquad (9.47)$$

and the time-independent Schrödinger equation for this system appears as

$$\hat{H}\varphi = \left(\frac{\hat{L}^2}{2I}\right)\varphi = E\varphi \qquad (9.48)$$

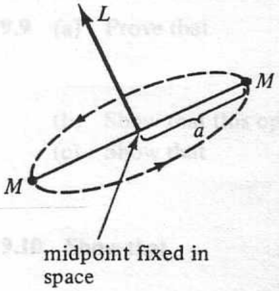


FIGURE 9.7 **Rigid rotator with fixed midpoint. Moment of inertia about midpoint is $I = 2Ma^2$.**

The eigenvalues of $\hat{H}$ are the same as those of the square angular momentum operator $\hat{L}^2$. With the results obtained we may rewrite the equation above with the l, m indices.

$$\left(\frac{\hat{L}^2}{2I}\right)\varphi_{lm} = E_l\varphi_{lm}$$

$$E_l = \frac{\hbar^2 l(l+1)}{2I} \tag{9.49}$$

This energy is $(2l + 1)$-fold degenerate. For any value of l, there are $(2l + 1)$ eigenfunctions

$$\varphi_{l,l}, \ldots, \varphi_{l,-l} = \{\varphi_{lm}\} \tag{9.50}$$

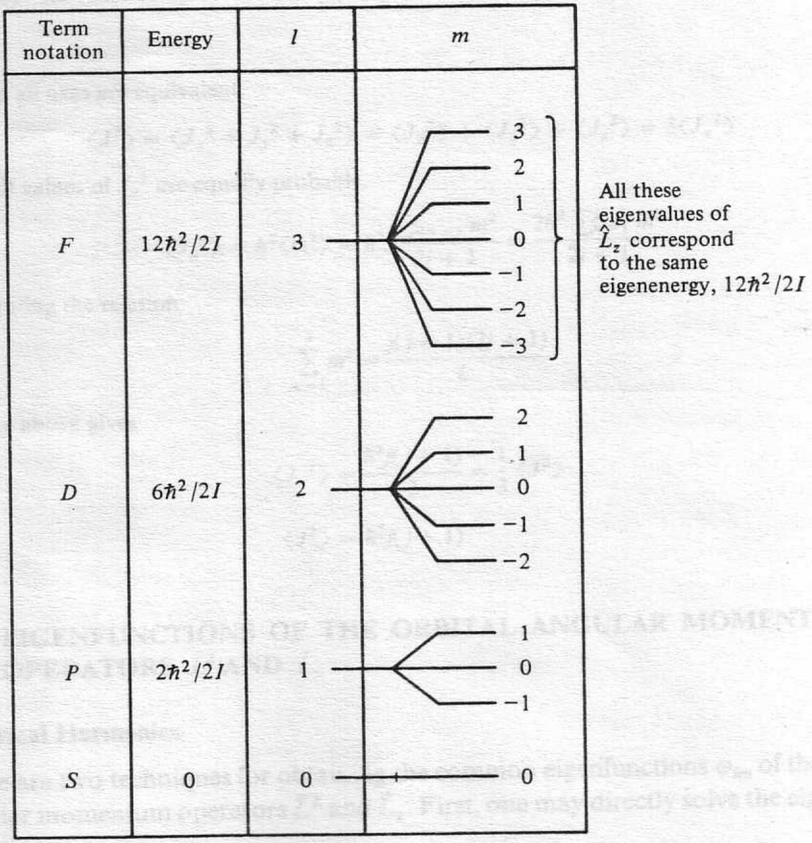


FIGURE 9.8 Term diagram for the rigid rotator of moment of inertia, I. The lth eigenenergy, $\hbar^2 l(l + 1)/2I$, is $(2l + 1)$-fold degenerate.

$\Rightarrow$ 1 $\hbar$ is Constant , 2 E_l is dependent on L and $I = 2Ma^2$

on the assumption that the mass of the rotator is Constant

but in general $E_l \equiv E_l(L, M, a)$ $\boxed{?}$, if $2M = m =$ Constant

3 $E_l =$ Constant when $L =$ Constant and a is Constant

$\rightarrow$ $a =$ Const $\rightarrow$ all kinds of orbitals (φ_{lm}) (motion) on a sphere are possible $\boxed{?}$

Hence the idea of Spherical Harmonics for $L =$ Const.

4 Can a and L be represented together in one Space

$a = |\underline{r}|$ (sphere radius) , $\hat{L} = \underline{e}_x \hat{L}_x + \underline{e}_y \hat{L}_y + \underline{e}_z \hat{L}_z$. $\boxed{\text{re-examine}}$ $\boxed{?}$

5 Yes, the rigid rotator describes a simple atomic system.

(9.5) $\hbar\omega = E_{l+1} - E_l = \frac{\hbar^2}{2I}\left((l+1)(l+2) - l(l+1)\right) = \frac{2}{2}\frac{\hbar^2}{I}(l+1)$,

$l^2 + 3l + 2 - l^2 - l = 2l + 2 = 2(l+1)$.

all corresponding to the same eigenenergy, (9.49). The energy of the rotator does not depend on the projection of **L** into the z axis or onto any other prescribed direction. The energy-level diagram for this system is sketched in Fig. 9.8, together with the "term notation" of levels. This notation is common to atomic spectroscopy and will be used in the next three chapters. When a particle is in a state of definite orbital angular momentum, characterized by the quantum number $l = 0, 1, 2, \ldots$, one speaks of the particle being respectively in an $S, P, D, F, \ldots$ state.

PROBLEMS

9.5 Show that the frequencies of photons due to energy decays between successive levels of a rotator with moment of inertia I are given by

$$\hbar\omega = \left(\frac{\hbar^2}{I}\right)(l+1)$$

9.6 An HCl molecule may rotate as well as vibrate. Discuss the difference in emission frequencies associated with these two modes of excitation. Assume that only $l \rightarrow l \pm 1$ transitions between rotational states are allowed. Spring constant and moment of inertia may be inferred from the equivalent temperature values for HCl: $\hbar\omega_0/k_B = 4150$ K; $\hbar^2/2Ik_B = 15.2$ K.

9.7 Show that

(a) $[\hat{L}_x, \hat{x}] = 0$ (f) $[\hat{p}_x, \hat{L}_x] = 0$
(b) $[\hat{L}_x, \hat{y}] = i\hbar\hat{z}$ (g) $[\hat{p}_x, \hat{L}_y] = i\hbar\hat{p}_z$
(c) $[\hat{L}_y, \hat{z}] = i\hbar\hat{x}$ (h) $[\hat{p}_y, \hat{L}_z] = i\hbar\hat{p}_x$
(d) $[\hat{L}_z, \hat{x}] = i\hbar\hat{y}$ (i) $[\hat{p}_z, \hat{L}_x] = i\hbar\hat{p}_y$
(e) $[\hat{L}_y, \hat{z}] = [\hat{y}, \hat{L}_z]$ (j) $[\hat{L}_y, \hat{p}_z] = [\hat{p}_y, \hat{L}_z]$

9.8 Calculate

(a) $\hat{L}_z kr$
(b) $\hat{L}_z \sin kr$
(c) $\hat{L}_z f(kr)$

explicitly in Cartesian coordinates, with $r^2 = x^2 + y^2 + z^2$. The function f is an arbitrary function of r, and k is a constant wavenumber.

9.9 (a) Prove that

$$\hat{\mathbf{\Theta}} \equiv \hat{\mathbf{L}} \times \hat{\mathbf{r}} - i\hbar\hat{\mathbf{r}} = i\hbar\hat{\mathbf{r}} - \hat{\mathbf{r}} \times \hat{\mathbf{L}}$$

(b) Show that this operator is Hermitian.
(c) Show that

$$[\hat{L}^2, \hat{\mathbf{r}}] = -2i\hbar\hat{\mathbf{\Theta}}$$

9.10 Show that

$$[\hat{L}_x{}^2, \hat{L}_y{}^2] = [\hat{L}_y{}^2, \hat{L}_z{}^2] = [\hat{L}_z{}^2, \hat{L}_x{}^2]$$

9.11 Evaluate

(a) $[\hat{L}^2, \hat{\mathbf{p}}]$ (c) $[\hat{\mathbf{L}}, \hat{p}^2]$

(b) $[\hat{\mathbf{L}}, \hat{\mathbf{p}}]$ (d) $[\hat{\mathbf{L}}, \hat{\mathbf{L}} \times \hat{\mathbf{L}}]$

Note that parts (b) and (d) have nine components. They are called *dyadic operators.*

9.12 Show that

$$[\hat{L}_x, \hat{r}^2] = [\hat{L}_y, \hat{r}^2] = [\hat{L}_z, \hat{r}^2] = 0$$

† **9.13** Show that the expression

$$\langle J^2 \rangle = \hbar^2 j(j+1)$$

is implied directly by the two assumptions:

(a) The only possible values that the components of angular momentum can have on any axis are $\hbar(-j, \ldots, +j)$.

(b) All these components are equally probable.

Answer

Because all axes are equivalent,

$$\langle J^2 \rangle = \langle J_x{}^2 + J_y{}^2 + J_z{}^2 \rangle = \langle J_x{}^2 \rangle + \langle J_y{}^2 \rangle + \langle J_z{}^2 \rangle = 3\langle J_x{}^2 \rangle$$

Since all values of $J_x{}^2$ are equally probable,

$$\langle J_x{}^2 \rangle = \hbar^2 \langle m^2 \rangle = \hbar^2 \frac{\sum_{m=-j}^{j} m^2}{2j+1} = \frac{2\hbar^2 \sum_{m=1}^{j} m^2}{2j+1}$$

Substituting the relation

$$\sum_{m=1}^{j} m^2 = \frac{j(j+1)(2j+1)}{6}$$

into the above gives

$$\langle J_x{}^2 \rangle = \frac{\hbar^2 j(j+1)}{3} = \frac{1}{3} \langle J^2 \rangle$$

$$\langle J^2 \rangle = \hbar^2 j(j+1)$$

9.3 EIGENFUNCTIONS OF THE ORBITAL ANGULAR MOMENTUM OPERATORS $\hat{L}^2$ AND $\hat{L}_z$

Spherical Harmonics

1st There are two techniques for obtaining the common eigenfunctions φ_{lm} of the orbital angular momentum operators $\hat{L}^2$ and $\hat{L}_z$. First, one may directly solve the eigenvalue equations

$$\begin{aligned} \hat{L}^2 \varphi_{lm} &= \hbar^2 l(l+1)\varphi_{lm} \\ \hat{L}_z \varphi_{lm} &= \hbar m \varphi_{lm} \end{aligned} \tag{9.51}$$

2nd Second, one may seek solution to the equation

$$\hat{L}_+ \varphi_{ll} = 0 \tag{9.52}$$

Once having found φ_{ll}, the remaining eigenfunctions of $\hat{L}^2$ and $\hat{L}_z$, corresponding to the orbital quantum number l,

$$\{\varphi_{lm}\} = (\varphi_{ll}, \varphi_{l,l-1}, \ldots, \varphi_{l,-l}) \tag{9.53}$$

are obtained by applying $\hat{L}_-$ to φ_{ll}. That is,

$$\begin{aligned} \varphi_{l,l-1} &= \hat{L}_- \varphi_{ll} \\ \varphi_{l,l-2} &= \hat{L}_- \varphi_{l,l-1} \end{aligned} \tag{9.54}$$

1 In either technique for obtaining the eigenfunctions φ_{lm}, it proves both convenient and practical to work in spherical coordinates (r, θ, ϕ) (see Fig. 1.6). These coordinates are related to the Cartesian coordinates (x, y, z) through the transformation equations

$$\begin{aligned} x &= r \sin\theta \cos\phi \\ y &= r \sin\theta \sin\phi \\ z &= r \cos\theta \end{aligned} \tag{9.55}$$

2 With these equations, the Cartesian components of $\hat{\mathbf{L}}$, (9.3), are transformed to (see Problem 9.14)

$$\begin{aligned} \hat{L}_x &= i\hbar\left(\sin\phi \frac{\partial}{\partial\theta} + \cot\theta\cos\phi \frac{\partial}{\partial\phi}\right) \\ \hat{L}_y &= i\hbar\left(-\cos\phi \frac{\partial}{\partial\theta} + \cot\theta\sin\phi \frac{\partial}{\partial\phi}\right) \\ L_z &= -i\hbar \frac{\partial}{\partial\phi} \end{aligned} \tag{9.56}$$

3 Using expressions (9.56) we obtain first the ladder operators

$$\begin{aligned} \hat{L}_+ &= \hat{L}_x + i\hat{L}_y = \hbar e^{i\phi}\left(i\cot\theta \frac{\partial}{\partial\phi} + \frac{\partial}{\partial\theta}\right) \\ \hat{L}_- &= \hat{L}_x - i\hat{L}_y = \hbar e^{-i\phi}\left(i\cot\theta \frac{\partial}{\partial\phi} - \frac{\partial}{\partial\theta}\right) \end{aligned} \tag{9.57}$$

4 and second, the operator $\hat{L}^2$

$$\hat{L}^2 = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right] \tag{9.58}$$

We are now prepared to seek solutions to (9.51). This is the first technique, as mentioned above, for finding the eigenstates φ_{lm}. These solutions are quite common to many branches of physics. They are called *spherical harmonics* and are universally denoted by the symbol Y_l^m. Following this protocol we change notation: $\varphi_{lm} \rightarrow Y_l^m$.

·2 Angular Momentum and Rotation

Before discussing these solutions we note two points. First, all the angular momentum operators, when expressed in spherical coordinates as listed above, are independent 1 of r. They are functions only of the angular variables (θ, ϕ). This means that the eigenfunctions of $\hat{L}^2$ and $\hat{L}_z$ may be chosen independent of r, that is, $Y_l^m = Y_l^m(\theta, \phi)$. 2 This property stems from the fact that angular momentum operators are related to rotation. For instance, the operator

$$\hat{R}_{\delta\boldsymbol{\phi}} = 1 + i\delta\boldsymbol{\phi} \cdot \frac{\mathbf{L}}{\hbar} \tag{9.59}$$

3 (described previously in Section 6.3) when acting on $f(\mathbf{r})$ rotates $\mathbf{r}$ through the azimuthal displacement $\delta\boldsymbol{\phi}$, so that

$$\begin{gathered} \hat{R}_{\delta\boldsymbol{\phi}} f(\mathbf{r}) = f(\mathbf{r} + \delta\mathbf{r}) \\ \delta\mathbf{r} = \delta\boldsymbol{\phi} \times \mathbf{r} \end{gathered} \tag{9.60}$$

1· So the effect of the operation $\delta\boldsymbol{\phi} \cdot \hat{\mathbf{L}}$ on a function $\mathbf{r}$ is to cause a rotational displace- 2· ment of $\mathbf{r}$. If $\delta\boldsymbol{\phi}$ is parallel to the z axis, $\delta\boldsymbol{\phi} \cdot \hat{\mathbf{L}} = \delta\phi L_z$. This operator induces a rotation of $\mathbf{r}$ about the z axis, without changing the magnitude of $\mathbf{r}$. 3· If we write $f(\mathbf{r}) = f(r, \theta, \phi)$, then $\hat{L}_z$ when operating on f affects only the variable ϕ. When L^2 operates on this function, θ and ϕ are both affected, but not r. So here we have the reason that the eigenstates of $\hat{L}^2$ and $\hat{L}_z$ may be chosen independent of r.

·3 Normalization

The second point we wish to note relates to the normalization of the Y_l^m functions. This normalization is taken over the surface of a unit sphere. 1 The differential element of area dS, on the surface of a sphere of radius a, is conveniently expressed in terms of the element of *solid angle* $d\Omega$.

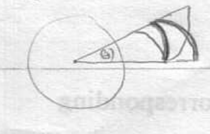
$$dS = a^2\, d\Omega = a^2 \sin\theta\, d\theta\, d\phi \tag{9.61}$$

2 (see Fig. 9.9). The solid angle subtended by dS about the origin is $dS/a^2 = d\Omega$. The solid angle subtended by a sphere (more generally any closed surface) about the origin is

$$\int_{\text{all directions}} d\Omega = \int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta\, d\theta = \int_0^{2\pi} d\phi \int_{-1}^{1} d\cos\theta = 4\pi \text{ steradians} \tag{9.62}$$

which is the same as the area of a unit sphere (a sphere of unit radius).

1 Integral Transforms (Convolution): $h(x) = \int_{-\infty}^{\infty} f(t)\, g(x-t)\, dt$

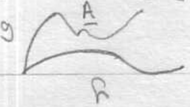
2 $\theta = \frac{S}{r}$ 

over a Circle $S = r\theta$, $dS = r\, d\theta$,

over a Sphere $S = r^2 \Omega$, $dS = r^2 d\Omega$

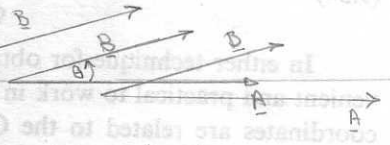
3

$\underline{A} \cdot \underline{B} = \sum_{\forall i} a_i b_i$ Projection of direction $\underline{B}$ over direction $\underline{A}$,

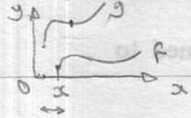
4 

projection of Curve g over another Curve f

$\longrightarrow \int_{\forall x} f(x)\, g(x)\, dx$ $\boxed{?}$



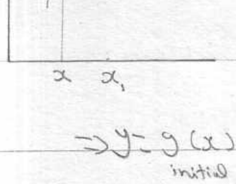
5 Vectors allow "Parallel displacement" without Changing magnitude or direction, what about functions i.e Curves?

6 

Can we bring g, by parallel displacement, to a Common "Point origin" x s.t we Can do the Projection ?

7 What is the relation between initial g and g after parallel displacement??

8 How this is related to $g(x-t)$ in 1 ? $\underline{x} = \underline{x}_1 + \underline{\alpha}$

9 

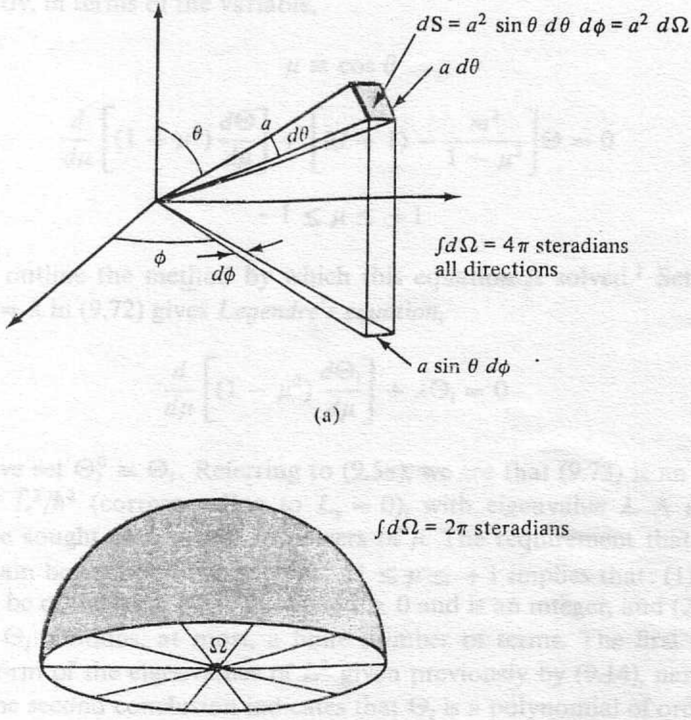
if $y = g$ is Preserved even after the displacement

$\Rightarrow \underline{\alpha} = (\alpha, \beta) = (\alpha, 0)$, $x_1 = x - \alpha$

$\Rightarrow \underset{\text{initial}}{y = g(x)} = \underset{\text{after P.d}}{g(x-\alpha)}$ $\boxed{?}$ is $t \sim \alpha$ $\boxed{?}$

Perhaps I misunderstood the Correspondence in 3, 4. (Mon. 31-8-1992)
(12.00 GMT)

Relate (9.64) to Time independent $\hat{H} = \hat{H}(r) \to \Psi(x,t) = \phi(x)\, T($


$dS = a^2 \sin\theta \, d\theta \, d\phi = a^2 \, d\Omega$
$a \, d\theta$
θ
a
$d\theta$
$\int d\Omega = 4\pi$ steradians
all directions
ϕ
$d\phi$
$a \sin\theta \, d\phi$
$\int d\Omega = 2\pi$ steradians
Ω

(a)

(b)

FIGURE 9.9 (a) Element of the solid angle $d\Omega = dS/a^2$. (b) Solid angle subtended by the hemisphere about the origin O is 2π.

To normalize the eigenfunctions Y_l^m, set

$$\int_{4\pi} |Y_l^m|^2 \, d\Omega = 1 \tag{9.63}$$

which we see is the same as requiring that $|Y_l^m|^2$ integrate to unity over the surface of a unit sphere.

We are now prepared to discuss the solutions to (9.51). The eigenfunction equation for $\hat{L}_z$ gives

$$\frac{\partial}{\partial\phi} Y_l^m = im Y_l^m \tag{9.64}$$

This equation determines only the ϕ dependence of Y_l^m. If we set

$$Y_l^m(\theta, \phi) = \Phi_m(\phi)\Theta_l^m(\theta) \tag{9.65}$$

3. the equation above gives

$$\Phi_m(\phi) = \frac{1}{\sqrt{2\pi}} e^{im\phi} \tag{9.66}$$

which satisfies the normalization

$$\int_0^{2\pi} d\phi \, |\Phi_m|^2 = 1 \tag{9.67}$$

1. The index m can be determined from the single valuedness[1] of the wavefunction Φ. That is

$$\begin{gathered} \Phi(\phi) = \Phi(\phi + 2\pi) \\ e^{im\phi} = e^{im(\phi + 2\pi)} \\ e^{im2\pi} = 1 \end{gathered} \tag{9.68}$$

which is only satisfied for integral values of m:

$$m = 0, 1, 2, \ldots \tag{9.69}$$

As demonstrated in Section 9.2 the values of m run from $-l$ to $+l$, whence l is also an integer. Thus we obtain the result stated previously that the l, m orbital angular momentum quantum numbers are integers only. We also see how this property follows directly from boundary conditions imposed on the wavefunctions Y_l^m. Spin, being an intrinsic property of a particle, is not so constrained, and the related quantum s numbers may assume half-odd-integral as well as integral values.

2.

Legendre Polynomials

We have found that the eigenfunction Y_l^m has the structure

$$Y_l^m = \frac{1}{\sqrt{2\pi}} e^{im\phi} \Theta_l^m(\theta) \tag{9.70}$$

1 Substituting this function into (9.51), together with the explicit expression for $\hat{L}^2$ as given by (9.58), gives the following equation for Θ_l^m (deleting l and m indices, for the moment):

$$\frac{1}{\sin\theta} \frac{d}{d\theta} \left(\sin\theta \frac{d\Theta}{d\theta} \right) + \left[l(l+1) - \frac{m^2}{\sin^2\theta} \right] \Theta = 0 \tag{9.71}$$

---

[1] On physical grounds it is more appropriate to require that $|\Phi|^2$ be single valued. However, this can be shown to be equivalent to the single valuedness of Φ for the case in point. For further discussion, see K. Gottfried, *Quantum Mechanics*, W. A. Benjamin, New York, 1966.

1· or equivalently, in terms of the variable,

$$\mu \equiv \cos\theta$$

$$\frac{d}{d\mu}\left[(1-\mu^2)\frac{d\Theta}{d\mu}\right] + \left[l(l+1) - \frac{m^2}{1-\mu^2}\right]\Theta = 0 \tag{9.72}$$

$$-1 \le \mu \le +1$$

2 Let us outline the method by which this equation is solved.[1] Setting $m = 0$ and $l(l+1) = \lambda$ in (9.72) gives *Legendre's equation*,

$$\frac{d}{d\mu}\left[(1-\mu^2)\frac{d\Theta_l}{d\mu}\right] + \lambda\Theta_l = 0 \tag{9.73}$$

where we have set $\Theta_l^0 \equiv \Theta_l$. Referring to (9.58), we see that (9.73) is an eigenvalue
equation for $\hat{L}^2/\hbar^2$ (corresponding to $L_z = 0$), with eigenvalue λ. A solution to
3 (9.73) may be sought as a series[2] in powers of μ. The requirement that this series
solution remain bounded in the interval $-1 \le \mu \le +1$ implies that: (1) the eigen-
value λ must be of the form $l(l+1)$, where $l \ge 0$ and is an integer, and (2) the series
solution for Θ_l contains, at most, a finite number of terms. The first conclusion
3· returns the form of the eigenvalues of L^2 given previously by (9.14), namely, $L^2 =$
$\hbar^2 l(l+1)$. The second conclusion indicates that Θ_l is a polynomial of order l. These
4 polynomials, called *Legendre polynomials*, are commonly denoted as $P_l(\mu)$, so that
apart from a multiplicative constant, $\Theta_l(\mu) = P_l(\mu)$. The series summation for this
solution may be expressed in the concise form, called the *formula of Rodrigues*,

$$P_l(\mu) = \frac{1}{2^l l!}\frac{d^l}{d\mu^l}(\mu^2-1)^l \tag{9.74}$$

·1 With this solution to (9.73) at hand, the solution to (9.72) is obtained by first constructing the *associated Legendre polynomials*. These are defined by[3] the following differential operation on $P_l(\mu)$:

$$P_l^{\,m}(\mu) = (-1)^m(1-\mu^2)^{m/2}\frac{d^m P_l(\mu)}{d\mu^m} \tag{9.75}$$

---

[1] For a more detailed description of this method of solution, see E. Merzbacher, *Quantum Mechanics*, 2nd ed., Wiley, New York, 1970. A closely related but more concise technique of solution is described in P. Stehle, *Quantum Mechanics*, Holden-Day, San Francisco, 1966.

[2] This method of series solution is explicitly demonstrated in Chapter 10 in the generation of Laguerre polynomials, which are components of the wavefunctions for the hydrogen atom.

[3] Another popular notation for these polynomials includes the $(-1)^m$ factor explicitly in the Y_l^m functions.

1 for positive integers $m \le l$. Differentiating Legendre's equation (9.73) m times with $\lambda = l(l+1)$, and Θ_l set equal to P_l, and employing the definition (9.75), one readily deduces the equation

$$\frac{d}{d\mu}\left[(1-\mu^2)\frac{dP_l^m}{d\mu}\right] + \left[l(l+1) - \frac{m^2}{1-\mu^2}\right]P_l^m = 0 \tag{9.76}$$

1· Comparison with (9.72) indicates that $P_l^m(\mu)$ is a solution to this same equation.
2 Furthermore, (9.72) remains unchanged if m is replaced by $-m$, and we may conclude that $P_l^{-m}(\mu)$ is also a solution to this equation, so that apart from a multiplicative constant, P_l^m is equal to P_l^{-m}.

3 In summary, we have found that the solutions $\Theta_l^m(\mu)$ to (9.72) are given by the associated Legendre polynomials $P_l^m(\mu)$. In addition, we see from the foregoing construction how the quantum conditions (9.14) emerge from the requirements that $Y_l^m(\Theta, \phi)$ remain nonsingular and single valued in the intervals $-1 \le \mu \le +1$, $0 \le \phi \le 2\pi$.

·2 The precise relation between $\Theta_l^m(\mu)$ and $P_l^m(\mu)$ as defined by (9.75) follows from the normalization condition (9.63).

$$\int_{4\pi} |Y_l^m|^2 \, d\Omega = \int_0^{2\pi} d\phi \left|\frac{e^{im\phi}}{\sqrt{2\pi}}\right|^2 \int_{-1}^{1} d\mu |\Theta_l^m(\mu)|^2 = 1$$

$$\int_{-1}^{1} d\mu |\Theta_l^m(\mu)|^2 = 1$$

1 There results

$$\Theta_l^m(\mu) = \left[\frac{2l+1}{2}\frac{(l-m)!}{(l+m)!}\right]^{1/2} P_l^m(\mu) \tag{9.77}$$

1· The first few spherical harmonics, Y_l^m, are listed in Table 9.1. Important properties of the Legendre polynomials, P_l, are listed in Table 9.2, while properties of the associated Legendre polynomials, P_l^m, are listed in Table 9.3.

3· Polar Plots of Y_l^m and Spherical Harmonic Expansions

When a system such as a rigid rotator is in an eigenstate of $\hat{L}^2$ and $\hat{L}_z$, the z axis is said to be *preferred*. Namely, measurement of L_z is certain to find a specific value.
1 However, in this state, it is still true that the x direction is in no way preferred over the
2 y direction. Thus the probability density, $|Y_l^m|^2$, is rotationally symmetric about the z axis or, equivalently (from 9.70), $|Y_l^m|$ is independent of ϕ. The function $|Y_l^m|$ is a surface of revolution about the z axis.

$$|Y_l^m| = \frac{1}{\sqrt{2\pi}}|\Theta_l^m(\cos\theta)| = \left[\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}\right]^{1/2} |P_l^m(\cos\theta)| \tag{9.78}$$

TABLE 9.1 The first few normalized spherical harmonics and corresponding associated Legendre polynomials[a]

$$Y_l^m(\theta, \phi) = \left[\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}\right]^{1/2} P_l^m(\cos\theta) e^{im\phi}$$

$$\int_{-1}^{1} d\cos\theta \int_0^{2\pi} d\phi \, Y_l^m (Y_{l'}^{m'})^* = \delta_{mm'}\delta_{ll'}$$

$$P_0 = 1$$

$$P_1{}^1 = -\sin\theta$$

$$P_1{}^0 = \cos\theta$$

$$P_1{}^{-1} = \tfrac{1}{2}\sin\theta$$

$$P_2{}^2 = 3\sin^2\theta$$

$$P_2{}^1 = -3\sin\theta\cos\theta$$

$$P_2{}^0 = \tfrac{1}{2}(3\cos^2\theta - 1)$$

$$P_2{}^{-1} = \tfrac{1}{2}\sin\theta\cos\theta$$

$$P_2{}^{-2} = \tfrac{1}{8}\sin^2\theta$$

$$P_3{}^3 = -15\sin^3\theta$$

$$P_3{}^2 = 15\sin^2\theta\cos\theta$$

$$P_3{}^1 = -\tfrac{3}{2}\sin\theta(5\cos^2\theta - 1)$$

$$P_3{}^0 = \tfrac{1}{2}(5\cos^3\theta - 3\cos\theta)$$

$$P_3{}^{-1} = \tfrac{1}{8}\sin\theta(5\cos^2\theta - 1)$$

$$P_3{}^{-2} = \tfrac{1}{8}\sin^2\theta\cos\theta$$

$$P_3{}^{-3} = \tfrac{1}{48}\sin^3\theta$$

$$Y_l{}^{-l} = \frac{1}{2^l l!}\sqrt{\frac{(2l+1)!}{4\pi}}\sin^l\theta e^{-il\phi}$$

$$Y_l{}^0 = \sqrt{\frac{2l+1}{4\pi}} P_l(\cos\theta)$$

$$\sum_{m=-l}^{l} |Y_l^m(\theta, \phi)|^2 = \frac{2l+1}{4\pi}$$

$$Y_l{}^{-m} = (-1)^m (Y_l^m)^*$$

$$Y_0{}^0 = \left(\frac{1}{4\pi}\right)^{1/2}$$

$$Y_1{}^1 = -\frac{1}{2}\left(\frac{3}{2\pi}\right)^{1/2} \sin\theta\, e^{i\phi}$$

$$Y_1{}^0 = \frac{1}{2}\left(\frac{3}{\pi}\right)^{1/2} \cos\theta$$

$$Y_1{}^{-1} = \frac{1}{2}\left(\frac{3}{2\pi}\right)^{1/2} \sin\theta e^{-i\phi}$$

$$Y_2{}^2 = \frac{1}{4}\left(\frac{15}{2\pi}\right)^{1/2} \sin^2\theta e^{2i\phi}$$

$$Y_2{}^1 = -\frac{1}{2}\left(\frac{15}{2\pi}\right)^{1/2} \sin\theta\cos\theta e^{i\phi}$$

$$Y_2{}^0 = \frac{1}{4}\left(\frac{5}{\pi}\right)^{1/2} (3\cos^2\theta - 1)$$

$$Y_2{}^{-1} = \frac{1}{2}\left(\frac{15}{2\pi}\right)^{1/2} \sin\theta\cos\theta e^{-i\phi}$$

$$Y_2{}^{-2} = \frac{1}{4}\left(\frac{15}{2\pi}\right)^{1/2} \sin^2\theta e^{-2i\phi}$$

$$Y_3{}^3 = -\frac{1}{8}\left(\frac{35}{\pi}\right)^{1/2} \sin^3\theta\, e^{3i\phi}$$

$$Y_3{}^2 = \frac{1}{4}\left(\frac{105}{2\pi}\right)^{1/2} \sin^2\theta\cos\theta e^{2i\phi}$$

$$Y_3{}^1 = -\frac{1}{8}\left(\frac{21}{\pi}\right)^{1/2} \sin\theta(5\cos^2\theta - 1)e^{i\phi}$$

$$Y_3{}^0 = \frac{1}{4}\left(\frac{7}{\pi}\right)^{1/2} (5\cos^3\theta - 3\cos\theta)$$

$$Y_3{}^{-1} = \frac{1}{8}\left(\frac{21}{\pi}\right)^{1/2} \sin\theta(5\cos^2\theta - 1)e^{-i\phi}$$

$$Y_3{}^{-2} = \frac{1}{4}\left(\frac{105}{2\pi}\right)^{1/2} \sin^2\theta\cos\theta e^{-2i\phi}$$

$$Y_3{}^{-3} = \frac{1}{8}\left(\frac{35}{\pi}\right)^{1/2} \sin^3\theta e^{-3i\phi}$$

---

[a] Defining relations for $P_l(\mu)$ and $P_l^{-m}(\mu)$ are given in Table 9.3. Comparison with other notations for the spherical harmonics and their related functions may be found in D. Park, *Introduction to the Quantum Theory*, 2nd ed., McGraw-Hill, New York, 1974.

TABLE 9.2 Properties of the Legendre polynomials

Generating Formulas

$$(1 - 2\mu s + s^2)^{-1/2} = \sum_{l=0}^{\infty} P_l(\mu) s^l$$

$$P_l(\mu) = \frac{1}{2^l l!} \frac{d^l}{d\mu^l} (\mu^2 - 1)^l \begin{cases} -1 \le \mu \le 1 \\ l = 0, 1, 2, 3, \ldots \end{cases}$$

Legendre's Equation

$$(1 - \mu^2) \frac{d^2 P_l(\mu)}{d\mu^2} - 2\mu \frac{dP_l(\mu)}{d\mu} + l(l+1) P_l(\mu) = 0$$

Recurrence Relations

$$(l+1) P_{l+1}(\mu) = (2l+1) \mu P_l(\mu) - l P_{l-1}(\mu)$$

$$(1 - \mu^2) \frac{d}{d\mu} P_l(\mu) = -l\mu P_l(\mu) + l P_{l-1}(\mu)$$

Normalization and Orthogonality

$$\begin{aligned} \int_{-1}^{1} P_l(\mu) P_m(\mu)\, d\mu &= \frac{2}{2l+1} \qquad (l = m) \\ &= 0 \qquad (l \neq m) \end{aligned}$$

The First Few Polynomials

$$\begin{array}{lll} P_0 = 1 & P_2 = \frac{1}{2}(3\mu^2 - 1) & P_4 = \frac{1}{8}(35\mu^4 - 30\mu^2 + 3) \\ P_1 = \mu & P_3 = \frac{1}{2}(5\mu^3 - 3\mu) & P_5 = \frac{1}{8}(63\mu^5 - 70\mu^3 + 15\mu) \end{array}$$

Special Values

$$P_l(\mu) = (-1)^l P_l(-\mu) \qquad P_l(1) = 1$$

Polar plots of these functions for $l = 0, 1, 2$, and all accompanying m values, in any plane through the z axis, are sketched in Fig. 9.10.

The functions $Y_l^m(\theta, \phi)$ are a basis of the Hilbert space of square-integrable functions $\varphi(\theta, \phi)$ defined on the unit sphere. Such functions may be normalized as follows.

$$\|\varphi(\theta, \phi)\|^2 = \langle \varphi | \varphi \rangle = \int_0^{2\pi} d\phi \int_{-1}^{1} d\cos\theta\, \varphi^* \varphi = 1 \tag{9.79}$$

1 The expansion of φ in spherical harmonics is given by

$$\varphi(\theta, \phi) = \sum_{l=0}^{\infty} \sum_{|m| \le l} a_{lm} Y_l^m(\theta, \phi) \tag{9.80}$$

2 The coefficient of expansion a_{lm} is given by the inner product,

$$a_{lm} = \langle Y_l^m | \varphi \rangle = \int_0^{2\pi} d\phi \int_{-1}^{1} d\cos\theta [Y_l^m(\theta, \phi)]^* \varphi(\theta, \phi) \tag{9.81}$$

TABLE 9.3 Properties of the associated Legendre polynomials

Definition

$$P_l^m(\mu) = (-1)^m(1-\mu^2)^{m/2}\frac{d^m}{d\mu^m}P_l(\mu); \quad P_l^0 = P_l$$

$$P_l^{-m}(\mu) = (-1)^m\frac{(l-m)!}{(l+m)!}P_l^m(\mu); \quad P_l^{-l} = \frac{1}{2^l l!}\sin^l\theta$$

For these equations, m is taken as ≥ 0. In the formulas below, however, m may be < 0 also; $l = 0, 1, 2, 3, \ldots$, $|m| \leq l$.

Differential Equation

$$(1-\mu^2)\frac{d^2P_l^m(\mu)}{d\mu^2} - 2\mu\frac{dP_l^m(\mu)}{d\mu} + \left[l(l+1) - \frac{m^2}{1-\mu^2}\right]P_l^m(\mu) = 0$$

Recurrence Relations

$$(2l+1)\mu P_l^m(\mu) = (l-m+1)P_{l+1}{}^m(\mu) + (l+m)P_{l-1}{}^m(\mu)$$

$$(2l+1)(1-\mu^2)^{1/2}P_l^m(\mu) = P_{l-1}{}^{m+1}(\mu) - P_{l+1}{}^{m+1}(\mu)$$

$$\begin{aligned}(1-\mu^2)\frac{dP_l^m(\mu)}{d\mu} &= (l+1)\mu P_l^m(\mu) - (l-m+1)P_{l+1}{}^m(\mu)\\ &= -l\mu P_l^m(\mu) + (l+m)P_{l-1}{}^m(\mu)\end{aligned}$$

$$\begin{aligned}(1-\mu^2)^{1/2}P_l^{m+1}(\mu) &= (l-m)\mu P_l^m(\mu) - (l+m)P_{l-1}{}^m(\mu)\\ &= -(l+m+1)P_l^m(\mu) + (l-m+1)P_{l+1}{}^m(\mu)\end{aligned}$$

Normalization and Orthogonality

$$\begin{aligned}\int_{-1}^{1} P_l^m(\mu)P_k^m(\mu)\,d\mu &= \frac{2}{2l+1}\frac{(l+m)!}{(l-m)!} \qquad (l = k)\\ &= 0 \qquad (l \neq k)\end{aligned}$$

Suppose that at a given instant a system (e.g., a rigid rotator) is in the state $\varphi(\theta, \phi)$. Then the probability that measurement of L^2 finds the value $\hbar^2 l(l+1)$ is

$$P[\hbar^2 l(l+1)] = \sum_{m=-l}^{+l} |a_{lm}|^2 \tag{9.82}$$

while the probability of finding L_z with the value $\hbar m$ is

$$P(\hbar m) = \sum_{l=|m|}^{\infty} |a_{lm}|^2 \tag{9.83}$$

For example, consider that a rotator is in the state

$$\varphi(\theta, \phi) = A\sin^2\theta\cos 2\phi$$

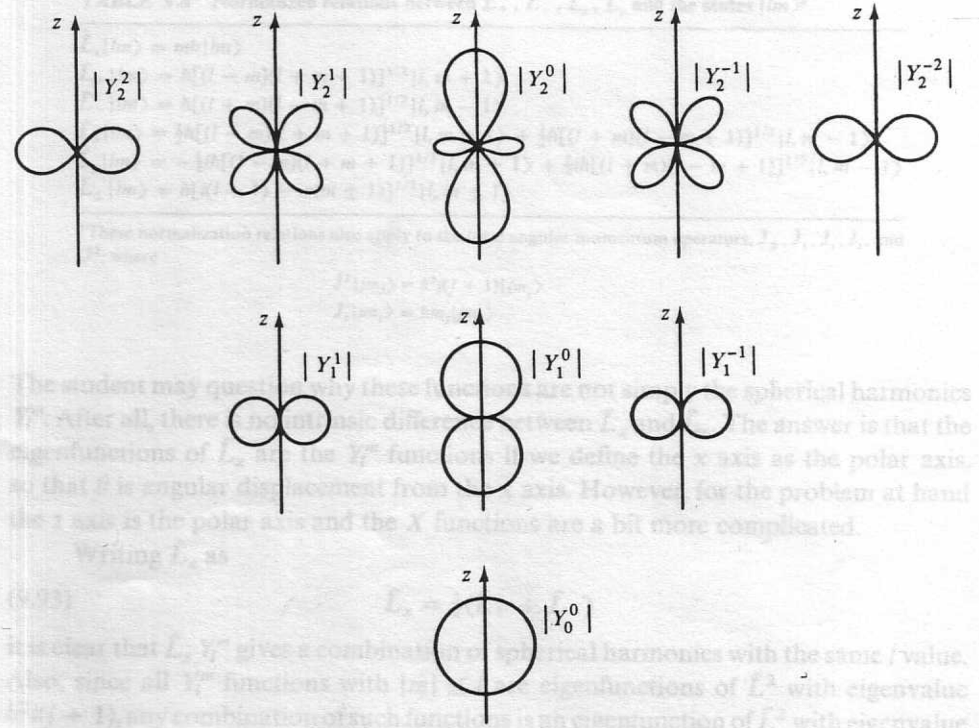


FIGURE 9.10 Polar plots of $|Y_l^m|$ versus θ in any plane through the z axis for $l = 0, 1, 2$. The equality $|Y_l^m| = |Y_l^{-m}|$ is exhibited.

2· What values of L^2 and L_z will measurement find? To answer this question, in principle
we should first evaluate the coefficients a_{lm} given by the operation (9.81). However,
3 for the case at hand, reference to Table 9.1 reveals that φ is the simple superposition

$$\varphi = A'(Y_2^{\,2} + Y_2^{\,-2})$$

3· where A and A' are constants. So the only coefficients that enter the expansion (9.80)
4 are a_{22} and a_{2-2}. We may conclude that measurement will find the value $L^2 = 6\hbar^2$
with probability 1 and the values $L_z = \pm 2\hbar$ with equal probabilities of $\frac{1}{2}$. No other
values of L_z and L^2 would be found for a rotator in the state given above.

4. Second Construction of the Spherical Harmonics

Let us now turn to the second procedure for finding the Y_l^m eigenfunctions, initiated by (9.52). Consider that we have already solved for the eigenfunction of $\hat{L}_z$, so that

φ_{lm} is known to be in the form given by (9.70). Equation (9.52) then becomes

$$\hat{L}_+ e^{il\phi}\Theta_l^{\,l}(\theta) = \hbar e^{i\phi}\left(\frac{\partial}{\partial\theta} + i\cot\theta\,\frac{\partial}{\partial\phi}\right)e^{il\phi}\Theta_l^{\,l}(\theta) = 0 \tag{9.84}$$

1 Bringing the exp $(il\phi)$ factor through the differential operator gives (deleting the l-scripts for the moment)

$$\frac{\partial}{\partial\theta}\Theta = l\cot\theta\,\Theta \tag{9.85}$$

1. Substituting the relation

$$l\cot\theta = \frac{\partial}{\partial\theta}\ln\sin^l\theta \tag{9.86}$$

2 and then dividing through by Θ gives

$$\frac{1}{\Theta}\frac{\partial}{\partial\theta}\Theta = \frac{\partial}{\partial\theta}\ln\Theta = \frac{\partial}{\partial\theta}\ln\sin^l\theta \tag{9.87}$$

This is simply integrated to yield

$$\Theta_l^{\,l} = A_{ll}\sin^l\theta \tag{9.88}$$

2. where A_{ll} is a normalization constant. It follows that Y_l^l is

$$Y_l^l = \frac{A_{ll}}{\sqrt{2\pi}}\sin^l\theta\, e^{il\phi} \tag{9.89}$$

3 which agrees with the values given in Table 9.1. The eigenfunction Y_l^{l-1} is obtained from Y_l^l through the operator $\hat{L}_-$.

$$\hat{L}_- Y_l^l = Y_l^{l-1} \tag{9.90}$$

In this manner we obtain

$$Y_l^{l-1} = A_{l,l-1}e^{i(l-1)\phi}\sin^{l-1}\theta\cos\theta \tag{9.91}$$

3. which is also in agreement with the values given in Table 9.1. The relations between $\hat{L}_+$, $\hat{L}_-$, and the Y_l^m functions with correct normalization factors are given in Table 9.4.

.1 We conclude this section with the following example. Suppose that a rigid rotator is in the eigenstate of $\hat{L}^2$ and $\hat{L}_z$ corresponding to $l = 1$ and $m = 1$ (i.e., $Y_1^{\,1}$). What is the probability that measurement of L_x finds the respective values $m = 0$,
1 ± 1? To answer this question we must expand $Y_1^{\,1}$ in the eigenfunctions of $\hat{L}_x$. These eigenfunctions are solutions to the equation

$$\hat{L}_x X(\theta,\phi) = \hbar\alpha X(\theta,\phi) \tag{9.92}$$

TABLE 9.4 Normalized relations between $\hat{L}_+$, $\hat{L}_-$, $\hat{L}_x$, $\hat{L}_y$ and the states $|lm\rangle$[a]

$$\hat{L}_z|lm\rangle = m\hbar|lm\rangle$$
$$\hat{L}_+|lm\rangle = \hbar[(l-m)(l+m+1)]^{1/2}|l, m+1\rangle$$
$$\hat{L}_-|lm\rangle = \hbar[(l+m)(l-m+1)]^{1/2}|l, m-1\rangle$$
$$\hat{L}_x|lm\rangle = \tfrac{1}{2}\hbar[(l-m)(l+m+1)]^{1/2}|l, m+1\rangle + \tfrac{1}{2}\hbar[(l+m)(l-m+1)]^{1/2}|l, m-1\rangle$$
$$\hat{L}_y|lm\rangle = -\tfrac{1}{2}i\hbar[(l-m)(l+m+1)]^{1/2}|l, m+1\rangle + \tfrac{1}{2}i\hbar[(l+m)(l-m+1)]^{1/2}|l, m-1\rangle$$
$$\hat{L}_\pm|lm\rangle = \hbar[l(l+1) - m(m\pm 1)]^{1/2}|l, m\pm 1\rangle$$

[a] These normalization relations also apply to the total angular momentum operators, $\hat{J}_\pm$, $\hat{J}_x$, $\hat{J}_y$, $\hat{J}_z$, and $\hat{J}^2$, where

$$\hat{J}^2|jm_j\rangle = \hbar^2 j(j+1)|jm_j\rangle$$
$$\hat{J}_z|jm_j\rangle = \hbar m_j|jm_j\rangle$$

† 2 The student may question why these functions are not simply the spherical harmonics Y_l^m. After all, there is no intrinsic difference between $\hat{L}_x$ and $\hat{L}_z$. The answer is that the eigenfunctions of $\hat{L}_x$ are the Y_l^m functions if we define the x axis as the polar axis, so that θ is angular displacement from the x axis. However, for the problem at hand the z axis is the polar axis and the X functions are a bit more complicated.

2' Writing $\hat{L}_x$ as

$$\hat{L}_x = \tfrac{1}{2}(\hat{L}_+ + \hat{L}_-) \tag{9.93}$$

it is clear that $\hat{L}_x Y_l^m$ gives a combination of spherical harmonics with the same l value. 3 Also, since all Y_l^m functions with $|m| \leq l$ are eigenfunctions of $\hat{L}^2$ with eigenvalue $\hbar^2 l(l+1)$, any combination of such functions is an eigenfunction of $\hat{L}^2$ with eigenvalue $\hbar^2 l(l+1)$.

4 With these properties in mind we seek a solution to (9.92) in the form

$$X = aY_1{}^1 + bY_1{}^0 + cY_1{}^{-1} \tag{9.94}$$

The problem of finding the eigenfunctions of $\hat{L}_x$ (corresponding to $l = 1$) is then reduced to finding the coefficients a, b, and c in the expression above.

:2 From the properties of $\hat{L}_+$ and $\hat{L}_-$ listed in Table 9.4, we have

$$\begin{aligned} \hat{L}_+ Y_1{}^0 &= \sqrt{2}\hbar Y_1{}^1 \\ \hat{L}_+ Y_1{}^{-1} &= \sqrt{2}\hbar Y_1{}^0 \\ \hat{L}_- Y_1{}^0 &= \sqrt{2}\hbar Y_1{}^{-1} \\ \hat{L}_- Y_1{}^1 &= \sqrt{2}\hbar Y_1{}^0 \end{aligned} \tag{9.95}$$

1 Substituting the expansion (9.94) into the eigenvalue equation (9.92) and using the relations above gives the equation

$$(aY_1{}^0 + bY_1{}^1 + bY_1{}^{-1} + cY_1{}^0) = \sqrt{2}\alpha(aY_1{}^1 + bY_1{}^0 + cY_1{}^{-1}) \tag{9.96}$$

2 Since the Y_l^m functions form a linearly independent sequence, it follows that the only way to guarantee equality for all values of θ and ϕ in the equation above is to set the

coefficients of individual Y_l^m functions equal to zero. This gives the following set of three homogeneous algebraic equations:

$$\begin{pmatrix} -\sqrt{2}\alpha & 1 & 0 \\ 1 & -\sqrt{2}\alpha & 1 \\ 0 & 1 & -\sqrt{2}\alpha \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = 0 \tag{9.97}$$

3 A nontrivial solution of these equations occurs only for values of α that make the determinant of the coefficient matrix vanish. Setting the determinant equal to zero, one obtains

$$\alpha(\alpha^2 - 1) = 0 \tag{9.98}$$

which gives the eigenvalues

$$\alpha = 0, \qquad \alpha = 1, \qquad \alpha = -1 \tag{9.99}$$

·3 Substituting these values back into (9.97) gives the (normalized) eigenvectors

$$\begin{aligned} X_0 &= \frac{1}{\sqrt{2}}(Y_1{}^1 - Y_1{}^{-1}), && \alpha = 0 \\ X_+ &= \tfrac{1}{2}(Y_1{}^1 + \sqrt{2}\,Y_1{}^0 + Y_1{}^{-1}), && \alpha = +1 \\ X_- &= \tfrac{1}{2}(Y_1{}^1 - \sqrt{2}\,Y_1{}^0 + Y_1{}^{-1}), && \alpha = -1 \end{aligned} \tag{9.100}$$

1 With these eigenfunctions of $\hat{L}_x$ at hand it becomes a matter of inspection to construct the linear combination that gives $Y_1{}^1$. It is given by

$$Y_1{}^1 = \tfrac{1}{2}(X_+ + \sqrt{2}X_0 + X_-) \tag{9.101}$$

2 It follows that if the rotator is in the eigenstate of $\hat{L}^2$ and $\hat{L}_z$ corresponding to $l = 1$, $m = 1$, then the probability that measurement of L_x finds the value $+\hbar$ is $\frac{1}{4}$, the probability of finding $-\hbar$ is $\frac{1}{4}$, and the probability of finding 0 is $\frac{2}{4}$ (Fig. 9.11).

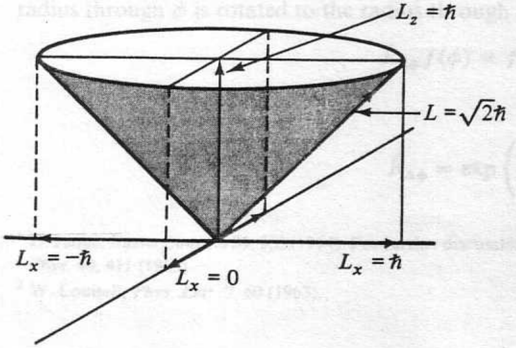


FIGURE 9.11 Given the state $L^2 = 2\hbar^2$, $L_z = \hbar$, what is the probability that measurement of L_x finds the values $\pm\hbar$, 0? Geometrical construction shows that two projections of **L** give $L_x = 0$, while one projection gives $L_x = +\hbar$ and one projection gives $L_x = -\hbar$.

PROBLEMS

9.14 Use transformation equations (9.55) to obtain the expression

$$\hat{L}_z = -i\hbar \frac{\partial}{\partial \phi}$$

Answer

From (9.55) we obtain the following useful relations.

$$r^2 = x^2 + y^2 + z^2, \qquad \cos\theta = \frac{z}{r}, \qquad \tan\phi = \frac{y}{x}$$

$$\frac{\partial \theta}{\partial x} = \frac{\cos\phi\cos\theta}{r} \qquad\qquad \frac{\partial \phi}{\partial x} = -\frac{y}{x^2}\cos^2\phi$$

$\nabla\theta$ $\qquad$ $\nabla\phi$

$$\frac{\partial \theta}{\partial y} = \frac{\sin\phi\cos\theta}{r} \qquad\qquad \frac{\partial \phi}{\partial y} = \frac{\cos^2\phi}{x}$$

$$\frac{\partial \theta}{\partial z} = -\frac{\sin\theta}{r} \qquad\qquad \frac{\partial \phi}{\partial z} = 0$$

∇r

$$\frac{\partial r}{\partial x} = \frac{x}{r}, \qquad \frac{\partial r}{\partial y} = \frac{y}{r}, \qquad \frac{\partial r}{\partial z} = \frac{z}{r}$$

For example, from $\cos\theta = z/r$, one obtains

$$-\sin\theta\frac{\partial\theta}{\partial x} = z\frac{\partial}{\partial x}\frac{1}{r} = -\frac{zx}{r^3} = -\frac{(z/r)(x/r)}{r} = -\frac{\cos\theta\sin\theta\cos\phi}{r}$$

Substituting these expressions in the expansion

$$\begin{aligned}\hat{L}_z &= -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)\\ &= -i\hbar\left[x\left(\frac{\partial\theta}{\partial y}\frac{\partial}{\partial\theta} + \frac{\partial\phi}{\partial y}\frac{\partial}{\partial\phi} + \frac{\partial r}{\partial y}\frac{\partial}{\partial r}\right) - y\left(\frac{\partial\theta}{\partial x}\frac{\partial}{\partial\theta} + \frac{\partial\phi}{\partial x}\frac{\partial}{\partial\phi} + \frac{\partial r}{\partial x}\frac{\partial}{\partial r}\right)\right]\end{aligned}$$

gives the desired result.

9.15 (a) What is $[\hat{\phi}, \hat{L}_z]$?

(b) Calculate the root-mean-square deviation $\Delta\phi$ for a particle in the uniform state $\varphi = 1/\sqrt{2\pi}$. (*Hint:* Perform your integrals over the interval $-\pi, \pi$.)

(c) Write down an uncertainty relation seemingly implied by your answer to part (a) and argue the physical inconsistency of this relation in view of your answer to part (b).

Answers

(a) $[\hat{\phi}, \hat{L}_z] = i\hbar$

(b) $\Delta\phi|_{\max} = \pi/\sqrt{3}$

(c) One is tempted to write $\Delta\phi\,\Delta L_z \geq \hbar/2$; however, by virtue of the result in part (b), uncertainty in ϕ greater than $\pi/\sqrt{3}$ has little physical meaning. In the extreme that the system is in an eigenstate (e.g., Y_l^m) of $\hat{L}_z$, $\Delta L_z = 0$ and the uncertainty relation gives $\Delta\phi = \infty$. Thus we may conclude that the assumed uncertainty relation is erroneous. [*Note:* Consider the space of functions $\mathfrak{H}_\phi$ whose elements have finite norm on the finite interval $(0, 2\pi)$ (i.e., $\int_0^{2\pi} \varphi^*\varphi \, d\phi < \infty$). It has been pointed out by D. Judge[1] that $\hat{L}_z$ is not Hermitian on this space. As a consequence, the derivation of the uncertainty relation between ϕ and $\hat{L}_z$ from their commutator relation fails. The non-Hermiticity of $\hat{L}_z$ on $\mathfrak{H}_\phi$ may be seen as follows. It is evident that the Hermiticity condition $\langle \hat{L}_z\varphi_1 | \varphi_2 \rangle = \langle \varphi_1 | \hat{L}_z \varphi_2 \rangle$ is valid only on the subspace $\mathfrak{H}_\phi' \subset \mathfrak{H}_\phi$ whose elements are periodic: $\varphi(0) = \varphi(2\pi)$. Hence $\hat{L}_z$ is non-Hermitian on $\mathfrak{H}_\phi$. Specifically, note that even though $\varphi(\phi)$ is periodic, the product $\phi\varphi(\phi)$ is not periodic and one may not invoke Hermiticity of $\hat{L}_z$ with respect to functions of this type. This is the crux of the breakdown in the proof of the uncertainty relation. See Problem 5.42.]

9.16 In regard to inconsistencies presented by the azimuthal angle ϕ, as discussed in Problem 9.15, it has been pointed out by W. Louisell[2] that more consistent angle variables are $\sin\phi$ and $\cos\phi$.

(a) Show that

$$[\sin\phi, \hat{L}_z] = i\hbar\cos\phi$$
$$[\cos\phi, \hat{L}_z] = -i\hbar\sin\phi$$

(b) Use these commutator formulas to obtain uncertainty relations between $\sin\phi$, L_z and $\cos\phi$, L_z.

Answer (*partial*)

(b)
$$\Delta L_z \, \Delta\sin\phi \geq \frac{\hbar\langle\cos\phi\rangle}{2}$$

$$\Delta L_z \, \Delta\cos\phi \geq \frac{\hbar\langle\sin\phi\rangle}{2}$$

9.17 (a) Show that the operator

$$\hat{R}_{\Delta\phi} \equiv \exp\left(\frac{i\,\Delta\phi\hat{L}_z}{\hbar}\right)$$

when acting on the function $f(\phi)$ changes f by a rotation of coordinates about the z axis so that the radius through ϕ is rotated to the radius through $\phi + \Delta\phi$. That is, show that

$$\hat{R}_{\Delta\phi} f(\phi) = f(\phi + \Delta\phi)$$

(b) Show that the operator

$$\hat{R}_{\Delta\boldsymbol{\phi}} = \exp\left(\frac{i\,\Delta\boldsymbol{\phi}\cdot\hat{\mathbf{L}}}{\hbar}\right)$$

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[1] D. Judge, *Nuovo Cimento* **31**, 332 (1964). For further discussion and reference, see P. Carruthers and N. Nieto, *Rev. Mod. Phys.* **40**, 411 (1968).

[2] W. Louisell, *Phys. Lett.* **7**, 60 (1963).

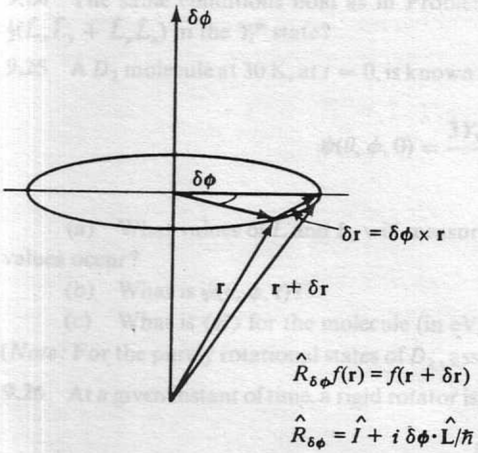
δφ
δφ
δr = δφ × r
r
r + δr
$\hat{R}_{\delta\phi} f(\mathbf{r}) = f(\mathbf{r} + \delta\mathbf{r})$
$\hat{R}_{\delta\phi} = \hat{I} + i\,\delta\boldsymbol{\phi}\cdot\hat{\mathbf{L}}/\hbar$

FIGURE 9.12 The rotation operator $\hat{R}_{\delta\phi}$ changes $f(\mathbf{r})$ by rotating r through the azimuthal increment $\delta\boldsymbol{\phi}$. See Problem 9.17.

when acting on $f(\mathbf{r})$ changes f by rotating $\mathbf{r}$ to a new value on the surface of the sphere of radius r, but rotated away from $\mathbf{r}$ through the azimuth $\Delta\phi$, so that $\mathbf{r}(\theta, \phi) \to \mathbf{r}' = \mathbf{r}(\theta, \phi + \Delta\phi)$. For infinitesimal displacements $\delta\boldsymbol{\phi}$, we may write

$$\hat{R}_{\delta\boldsymbol{\phi}} f(\mathbf{r}) = f(\mathbf{r} + \delta\mathbf{r})$$

$$\delta\mathbf{r} = \delta\boldsymbol{\phi} \times \mathbf{r}$$

See Fig. 9.12.

Answers

(a) $$\hat{R}_{\Delta\phi} f = \left[\exp\left(\Delta\phi\,\frac{\partial}{\partial\phi}\right)\right] f$$

$$= f(\phi) + \Delta\phi\,\frac{\partial f}{\partial\phi} + \frac{(\Delta\phi)^2}{2}\,\frac{\partial^2 f}{\partial\phi^2} + \cdots = f(\phi + \Delta\phi)$$

(b) Let $\delta\phi$ be an infinitesimal angle so that $\Delta\phi = n\delta\phi$ in the limit that $n \gg 1$. For the infinitesimal rotation

$$\mathbf{r}' = \mathbf{r} + \delta\mathbf{r} = \mathbf{r} + \delta\boldsymbol{\phi} \times \mathbf{r}$$

so that

$$\begin{aligned} f(\mathbf{r} + \delta\mathbf{r}) &= f(\mathbf{r}) + \delta\boldsymbol{\phi} \times \mathbf{r}\cdot\nabla f(\mathbf{r}) \\ &= f(\mathbf{r}) + \delta\boldsymbol{\phi}\cdot\mathbf{r} \times \nabla f(\mathbf{r}) \\ &= f(\mathbf{r}) + \frac{i}{\hbar}\,\delta\boldsymbol{\phi}\cdot\mathbf{r} \times \hat{\mathbf{p}} f(\mathbf{r}) \\ &= f(\mathbf{r}) + \frac{i}{\hbar}\,\delta\boldsymbol{\phi}\cdot\hat{\mathbf{L}} f(\mathbf{r}) \end{aligned}$$

In the Taylor series expansion of $f(\mathbf{r} + \delta\mathbf{r})$ above we have only kept terms of $O(\delta\phi)$. [The expression $\delta\mathbf{r} = \delta\boldsymbol{\phi} \times \mathbf{r}$ is valid only to terms of $O(\delta\phi)$.] In this manner we obtain

$$f(\mathbf{r} + \delta\mathbf{r}) = \left(\hat{I} + \frac{i}{\hbar}\,\delta\boldsymbol{\phi}\cdot\hat{\mathbf{L}}\right) f(\mathbf{r}) = \hat{R}_{\delta\boldsymbol{\phi}}\, f(\mathbf{r})$$

For a finite rotational displacement through the angle $\Delta\boldsymbol{\phi} = n\delta\boldsymbol{\phi}$, we apply the operator $\hat{R}_{\delta\boldsymbol{\phi}}$, n times:

$$\hat{R}_{n\delta\boldsymbol{\phi}} = (\hat{R}_{\delta\boldsymbol{\phi}})^n = \left(\hat{I} + \frac{i}{\hbar}\,\delta\boldsymbol{\phi}\cdot\hat{\mathbf{L}}\right)^n$$

and pass to the limit $n \rightarrow \infty$ or, equivalently, $\Delta\phi/\delta\phi \rightarrow \infty$.

$$\hat{R}_{\Delta\phi} = \lim_{\Delta\phi/\delta\phi\rightarrow\infty} \left(\hat{I} + \frac{i}{\hbar}\,\delta\boldsymbol{\phi}\cdot\hat{\mathbf{L}}\right)^{\Delta\phi/\delta\phi} = e^{i\Delta\boldsymbol{\phi}\cdot\hat{\mathbf{L}}/\hbar}$$

(*Note:* The operator $\hat{R}_{\delta\boldsymbol{\phi}}$ rotates $\mathbf{r}$ to $\mathbf{r} + \delta\boldsymbol{\phi} \times \mathbf{r}$ with respect to a fixed coordinate frame. If, on the other hand, the coordinate frame is rotated through $\delta\boldsymbol{\phi}$ with $\mathbf{r}$ fixed in space, then in the new coordinate frame this vector has the value $\mathbf{r} - \delta\boldsymbol{\phi} \times \mathbf{r}$. Thus, rotation of coordinates through $\delta\boldsymbol{\phi}$ is generated by the operator $\hat{R}_{-\delta\boldsymbol{\phi}}$.)

9.18 Show that $\hat{L}^2$ may be written as

$$\hat{L}^2 = -\hbar^2\left(\frac{\partial^2}{\partial\theta^2} + \cot\theta\,\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right)$$

9.19 Show by direct operation that

$$\hat{L}^2 Y_2{}^2 = 6\hbar^2 Y_2{}^2$$

$$\hat{L}_z Y_2{}^2 = 2\hbar Y_2{}^2$$

9.20 First calculate $P_2(\mu)$ using the generating function $(1 - 2\mu s + s^2)^{-1/2}$. Then obtain $P_2{}^1(\mu)$ using the relation between P_l and $P_l{}^m$ given in Table 9.3. Having found $P_2{}^1$, form $\Theta_2{}^1$ and then $Y_2{}^1$. Check your answers with the values given in Table 9.1.

9.21 Using the explicit form of $Y_l{}^m$, show that

$$\langle Y_l{}^m | Y_{l'}{}^{m'}\rangle = \langle lm | l'm'\rangle = 0 \qquad m \neq m'$$

9.22 Operate on $Y_l{}^{l-1}$ with $\hat{L}_-$ to obtain the angular dependent factor of $Y_l{}^{l-2}$.

9.23 Assume that a particle has an orbital angular momentum with z component $\hbar m$ and square magnitude $\hbar^2 l(l+1)$.

(a) Show that in this state

$$\langle L_x\rangle = \langle L_y\rangle = 0$$

(b) Show that

$$\langle L_x{}^2\rangle = \langle L_y{}^2\rangle = \frac{\hbar^2 l(l+1) - m^2\hbar^2}{2}$$

[*Hints:* For (a), use $\hat{L}_+$ and $\hat{L}_-$. For (b), use $\hat{L}^2 = \hat{L}_x{}^2 + \hat{L}_y{}^2 + \hat{L}_z{}^2$.]

9.24 The same conditions hold as in Problem 9.23. What is the expectation of the operator $\frac{1}{2}(\hat{L}_x\hat{L}_y + \hat{L}_y\hat{L}_x)$ in the Y_l^m state?

9.25 A D_2 molecule at 30 K, at $t = 0$, is known to be in the state

$$\psi(\theta, \phi, 0) = \frac{3Y_1{}^1 + 4Y_7{}^3 + Y_7{}^1}{\sqrt{26}}$$

(a) What values of L and L_z will measurement find and with what probabilities will these values occur?

(b) What is $\psi(\theta, \phi, t)$?

(c) What is $\langle E \rangle$ for the molecule (in eV) at $t > 0$?

(*Note*: For the purely rotational states of D_2, assume that $\hbar/2Ic = 30.4 \text{ cm}^{-1}$.)

9.26 At a given instant of time, a rigid rotator is in the state

$$\varphi(\theta, \phi) = \sqrt{\frac{3}{4\pi}} \sin\phi \sin\theta$$

(a) What possible values of L_z will measurement find and with what probability will these values occur?

(b) What is $\langle \hat{L}_x \rangle$ for this state?

(c) What is $\langle \hat{L}^2 \rangle$ for this state?

9.27 Suppose that a rotator is in the state $Y_1{}^{-1}$. What values will measurement of $\hat{L}_x$ find and with what probability will these values occur? (*Hint*: Most of the analysis in the text [(9.92) et seq.] involving the expansion of the state $Y_1{}^1$ may be used here.)

9.28 A one-particle system is in the angular state Y_l^m. Measurement is made of the component of **L** along the z' axis. The z' axis makes an angle λ with the z axis. What is the expectation of this component? What is the expectation of the square of this component? (See Fig. 9.13.)

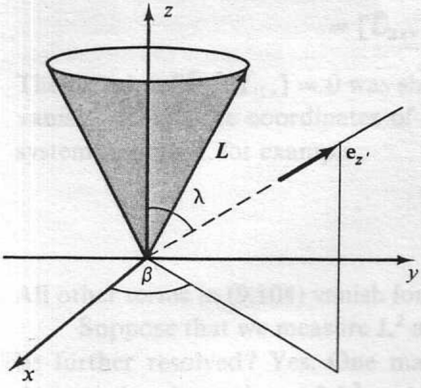

FIGURE 9.13 Configuration relevant to Problem 9.28.

Answer

For the first problem we must calculate $\langle \mathbf{e}_{z'} \cdot \hat{\mathbf{L}} \rangle$, where $\mathbf{e}_{z'}$ is the unit vector in the direction of the z' axis. For the second problem, we must calculate $\langle (\mathbf{e}_{z'} \cdot \hat{\mathbf{L}})^2 \rangle$. The components of $\mathbf{e}_{z'}$ are

$$\mathbf{e}_{z'} = (\sin\lambda\cos\beta, \sin\lambda\sin\beta, \cos\lambda)$$

where β is the azimuthal coordinate of $\mathbf{e}_{z'}$ with respect to the original axes.

$$\langle \mathbf{e}_{z'} \cdot \hat{\mathbf{L}} \rangle = \sin\lambda\cos\beta \langle L_x \rangle + \sin\lambda\sin\beta \langle L_y \rangle + \cos\lambda \langle L_z \rangle = \hbar m \cos\lambda$$

$$\langle (\mathbf{e}_{z'} \cdot \hat{\mathbf{L}})^2 \rangle = \sin^2\lambda \langle L_x{}^2 \rangle + \cos^2\lambda \langle L_z{}^2 \rangle$$

9.29 With $\Theta_l(\mu)$ replaced by $P_l(\mu)$ in (9.73), show that single differentiation of this equation gives (9.72) with $\Theta(\mu) = P_l{}^1(\mu)$ and $m = 1$.

9.4 ADDITION OF ANGULAR MOMENTUM

Two Electrons

In this section we examine the relation between the angular momentum of a total system and that of its constituents. This problem is of practical importance in atomic and nuclear physics where one encounters systems of many particles (e.g., electrons, neutrons, protons, etc.). In many cases one is chiefly concerned with the resultant angular momentum of the atom or nucleus.

Consider two systems that are rotating about a common origin. They could be two rotators or two electrons in an atom (Fig. 9.14). We will speak in terms of an atom. If the angular momentum (neglecting spin) of the first electron is $\mathbf{L}_1$ and that

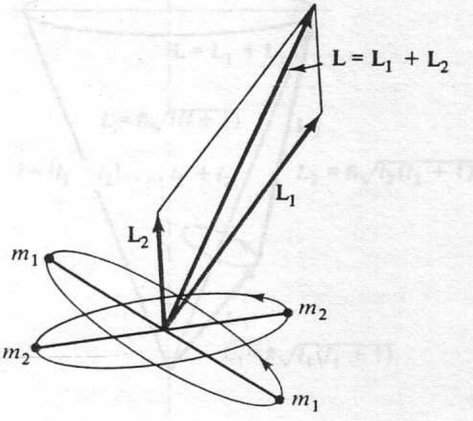

FIGURE 9.14 Classical addition of angular momentum. The two angular momentum vectors $\mathbf{L}_1$ and $\mathbf{L}_2$ add to give the resultant $\mathbf{L}$.

of the second electron is $\mathbf{L}_2$, the magnitude and z component of the total angular momentum of the composite system of the two electrons is

$$\hat{L}^2 = (\hat{\mathbf{L}}_1 + \hat{\mathbf{L}}_2)^2 = \hat{L}_1{}^2 + \hat{L}_2{}^2 + 2\hat{\mathbf{L}}_1 \cdot \hat{\mathbf{L}}_2 \qquad (9.102)$$
$$\hat{L}_z = \hat{L}_{1z} + \hat{L}_{2z}$$

2 Suppose that the total system is in a state with definite values of L_{1z}, L_{2z} (e.g., $|m_1 m_2\rangle$).
† 2· How much further may this state be resolved? Since there are only two good quantum numbers associated with each electron (i.e., $m_1 l_1$ and $m_2 l_2$), one suspects that the composite system will have no more than four good quantum numbers. As it turns out, the eigenstate $|m_1 m_2\rangle$ may further be resolved to the state $|l_1 l_2 m_1 m_2\rangle$.
3 This state cannot be further resolved. For instance, one might wish to measure L^2. If the atom is in the state $|l_1 l_2 m_1 m_2\rangle$ before measurement, we are not assured that it will be in that state after measurement of L^2. That this is so follows from the fact
3· that $\hat{L}^2$ does not commute with, say, $\hat{L}_{1z}$.

$$\begin{aligned} [\hat{L}_{1z}, \hat{L}^2] &= [\hat{L}_{1z}, \hat{L}_1{}^2 + \hat{L}_2{}^2 + 2\hat{\mathbf{L}}_1 \cdot \hat{\mathbf{L}}_2] \\ &= 2[\hat{L}_{1z}, \hat{\mathbf{L}}_1 \cdot \hat{\mathbf{L}}_2] = 2i\hbar(\hat{L}_{1y}\hat{L}_{2x} - \hat{L}_{1x}\hat{L}_{2y}) \end{aligned} \qquad (9.103)$$

·2 In order to establish that the set of eigenvalues (l_1, l_2, m_1, m_2) are *good quantum numbers* (i.e., that these values may be simultaneously specified in an eigenstate $|l_1 l_2 m_1 m_2\rangle$), one must show that the set of four operators $(\hat{L}_{1z}, \hat{L}_{2z}, \hat{L}_1{}^2, \hat{L}_2{}^2)$ are a set of mutually commuting operators. The fact that no other commuting operators
1 (restricting the discussion to the angular momentum properties of the system) can be attached to this set indicates that $(\hat{L}_{1z}, \hat{L}_{2z}, \hat{L}_1{}^2, \hat{L}_2{}^2)$ is a *complete* set of commuting operators.

We wish to show that

$$\begin{aligned} [\hat{L}_{1z}, \hat{L}_{2z}] &= [\hat{L}_{1z}, \hat{L}_1{}^2] = [\hat{L}_{1z}, \hat{L}_2{}^2] = [\hat{L}_{2z}, \hat{L}_1{}^2] \\ &= [\hat{L}_{2z}, \hat{L}_2{}^2] = [\hat{L}_1{}^2, \hat{L}_2{}^2] = 0 \end{aligned} \qquad (9.104)$$

2 The fact that $[\hat{L}_1{}^2, \hat{L}_{1z}] = 0$ was shown in Section 9.1. The commutators $[\hat{L}_{1z}, \hat{L}_{2z}]$ vanish because the coordinates of system 1 are independent of the coordinates of system 2, so that, for example,

$$\left[z_1, \frac{\partial}{\partial z_2}\right] = 0$$

All other terms in (9.104) vanish for similar reasons.

·3 Suppose that we measure L^2 and L_z and establish the state $|lm\rangle$. Can this state be further resolved? Yes. One may subsequently measure $L_1{}^2$ and $L_2{}^2$ and not destroy the eigenvalues of L^2 and L_z already established. After measurement, the system is left in the state $|lml_1l_2\rangle$. To show that l, m, l_1, and l_2 are good quantum numbers, we must establish that the set $(\hat{L}_1{}^2, \hat{L}_2{}^2, \hat{L}^2, \hat{L}_z)$ is a set of commuting operators. The only questionable pairs are of the form

$$[\hat{L}_1{}^2, \hat{L}^2] \quad \text{and} \quad [\hat{L}_1{}^2, \hat{L}_z]$$

Expanding these, we obtain

$$\begin{aligned} &[\hat{L}_1{}^2, \hat{L}_1{}^2 + \hat{L}_2{}^2 + 2\hat{\mathbf{L}}_1 \cdot \hat{\mathbf{L}}_2] = 2[\hat{L}_1{}^2, \hat{\mathbf{L}}_1 \cdot \hat{\mathbf{L}}_2] = 2[\hat{L}_1{}^2, \hat{\mathbf{L}}_1] \cdot \hat{\mathbf{L}}_2 = 0 \\ &[\hat{L}_1{}^2, \hat{L}_z] = [\hat{L}_1{}^2, \hat{L}_{1z} + \hat{L}_{2z}] = [\hat{L}_1{}^2, \hat{L}_{1z}] = 0 \end{aligned} \tag{9.105}$$

Coupled and Uncoupled Representations

Thus we find, in quantum mechanics, that the angular momentum states for a composite system consisting of two subsystems are characterized by either of two sets of good quantum numbers. These correspond, respectively, to the eigenstates $|l_1l_2m_1m_2\rangle$ and $|lml_1l_2\rangle$. The latter states pertain to problems where the total angular momentum of the composite system is important. We will call this representation where L^2 and L_z (together with $L_1{}^2$ and $L_2{}^2$) are specified the *coupled representation* (Fig. 9.15). The representation where the z component and magnitude of angular momentum are specified for all subcomponents (i.e., $L_1{}^2, L_{1z}, L_2{}^2, L_{2z}$) will be called the *uncoupled representation.*

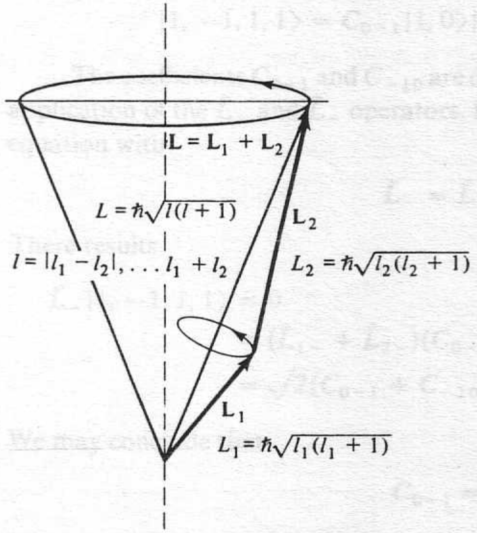
$\mathbf{L} = \mathbf{L}_1 + \mathbf{L}_2$
$L = \hbar\sqrt{l(l+1)}$
$l = |l_1 - l_2|, \ldots l_1 + l_2$
$\mathbf{L}_2$
$L_2 = \hbar\sqrt{l_2(l_2+1)}$
$\mathbf{L}_1$
$L_1 = \hbar\sqrt{l_1(l_1+1)}$

FIGURE 9.15 **In the coupled representation, $\mathbf{L}_1$ and $\mathbf{L}_2$ couple to give $\mathbf{L}$, which then exhibits discrete orientations along any prescribed axis. In this vector-model sketch of the state $|lml_1l_2\rangle$, the z components of $\mathbf{L}_1$ and $\mathbf{L}_2$ are not conserved. This corresponds to the fact that most generally, $|lml_1l_2\rangle$ is a superposition state involving all m_1, m_2 values with fixed $m_1 + m_2 = m$.**

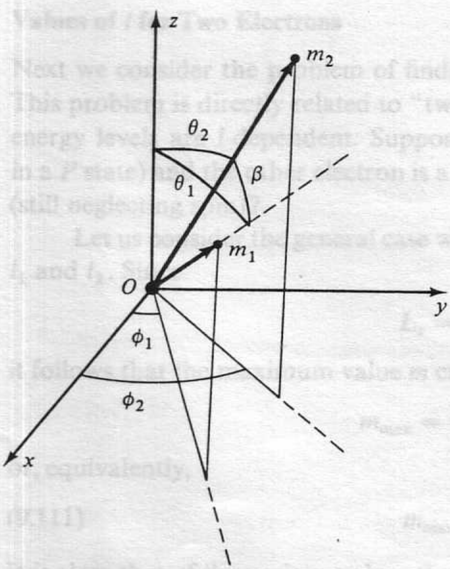

FIGURE 9.16 Angular coordinates for particle m_1 and particle m_2. Two important addition theorems involving the angle β between $0m_1$ and $0m_2$ are

(a) $$\cos\beta = \cos\theta_1\cos\theta_2 + \sin\theta_1\sin\theta_2\cos(\phi_1-\phi_2)$$

(b) $$P_l(\cos\beta) = \sum_{m=-l}^{l}\frac{(l-m)!}{(l+m)!} \times P_l^m(\cos\theta_1)P_l^m(\cos\theta_2)e^{im(\phi_1-\phi_2)} = \frac{2\pi}{2l+1} \times \sum_{m=-l}^{l}[Y_l^m(\theta_1,\phi_1)]^*Y_l^m(\theta_2,\phi_2)$$

·1 The eigenstates in either representation are constructed from products of the eigenstates $|m_1l_1\rangle$ and $|m_2l_2\rangle$. In the uncoupled representation the simultaneous eigenstates of $(\hat{L}_1{}^2, \hat{L}_{1z}, \hat{L}_2{}^2, \hat{L}_{2z})$ are given by the products

(9.106) $$|l_1l_2m_1m_2\rangle = |l_1m_1\rangle|l_2m_2\rangle$$

or, equivalently,

$$Y_{l_1}{}^{m_1}(\theta_1,\phi_1)Y_{l_2}{}^{m_2}(\theta_2,\varphi_2)$$

1 The spherical coordinates of electron 1 are θ_1, ϕ_1 while θ_2, ϕ_2 are the coordinates of 2 electron 2 (Fig. 9.16). For given values of l_1 and l_2 there are $(2l_1+1)(2l_2+1)$ linearly independent eigenstates of the composite system each of the form (9.106) and each with specified values of (l_1, l_2, m_1, m_2).

·2 Eigenstates $|lml_1l_2\rangle$ of the coupled representation are simultaneous eigenstates of the commuting operators

(9.107) $$\begin{gathered}\hat{L}^2 = \hat{L}_1{}^2 + \hat{L}_2{}^2 + 2\hat{\mathbf{L}}_1\cdot\hat{\mathbf{L}}_2\\ \hat{L}_z = \hat{L}_{1z} + \hat{L}_{2z}\\ \hat{L}_1{}^2, \hat{L}_2{}^2\end{gathered}$$

1 Any such state may be written as a superposition of the eigenstates of the uncoupled representation (9.106). In both representations l_1 and l_2 are good quantum numbers. 2 It follows that in the expansion

(9.108) $$|lml_1l_2\rangle = \sum_{m_1+m_2=m}\sum |l_1l_2m_1m_2\rangle\langle l_1l_2m_1m_2|lml_1l_2\rangle$$

summation can only run over the quantum numbers m_1 and m_2. The constraint
2· $m_1 + m_2 = m$ stems from the middle equation (9.107) and the orthogonality of
the states $|l_1 l_2 m_1 m_2\rangle$. Equation (9.108) may be rewritten

$$|lml_1l_2\rangle = \sum_{m_1+m_2=m}\sum C_{m_1m_2}|l_1l_2m_1m_2\rangle \tag{9.109}$$

$$C_{m_1m_2} \equiv \langle l_1l_2m_1m_2|lml_1l_2\rangle$$

3 The expansion coefficients $C_{m_1m_2}$ are called *Clebsch–Gordon* coefficients and their
significance is as follows. Let the composite system be two electrons. In the state
$|lml_1l_2\rangle$ it is known that these electrons have respective angular momentum quantum
numbers l_1 and l_2, and total angular momentum and z component quantum numbers
1 l and m. The question then arises as to what measurement of L_{1z} and L_{2z} will find
in the state $|lml_1l_2\rangle$. The answer to this question is that

$$|C_{m_1m_2}|^2 = \text{probability that measurement finds one electron with } L_{1z} = m_1\hbar \textit{ and } \text{the other electron with } L_{2z} = m_2\hbar \tag{9.110}$$

2 As an elementary illustration of the technique employed to construct these coefficients, let us consider expansion of the state

$$|lml_1l_2\rangle = |1, -1, 1, 1\rangle$$

With $m_1 + m_2 = -1$, the expansion (9.108) becomes

$$|1, -1, 1, 1\rangle = C_{0-1}|1, 0\rangle|1, -1\rangle + C_{-10}|1, -1\rangle|1, 0\rangle$$

+ 3 The coefficients C_{0-1} and C_{-10} are determined by normalization and propitious application of the $\hat{L}_+$ and $\hat{L}_-$ operators. For the case at hand, we operate on the last equation with

$$\hat{L}_- = \hat{L}_{1-} + \hat{L}_{2-}$$

There results

$$\begin{aligned} \hat{L}_-|1, -1, 1, 1\rangle = 0 & \\ &= (\hat{L}_{1-} + \hat{L}_{2-})(C_{0-1}|1, 0\rangle|1, -1\rangle + C_{-10}|1, -1\rangle|1, 0\rangle) \\ &= \sqrt{2}(C_{0-1} + C_{-10})|1, -1\rangle|1, -1\rangle \end{aligned}$$

3· We may conclude that

$$C_{0-1} = -C_{-10}$$

Normalization of the state $|1, -1, 1, 1\rangle$ gives $C_{0-1} = 1/\sqrt{2}$.

Values of l for Two Electrons

Next we consider the problem of finding the allowed values of (l, m), given (l_1, l_2). This problem is directly related to "two-electron atoms," such as He and Ca, whose energy levels are l-dependent. Suppose that one electron is a p-electron (i.e., it is in a P state) and the other electron is a d-electron. What values can result for l and m (still neglecting spin)?

Let us consider the general case where the two electrons have respective l values l_1 and l_2. Since

$$L_z = L_{1z} + L_{2z}$$

it follows that the maximum value m can have is

$$m_{\max} = m_{1_{\max}} + m_{2_{\max}}$$

or, equivalently,

$$m_{\max} = l_1 + l_2 \tag{9.111}$$

It is clear that of the various values the total angular momentum quantum number l may assume, the maximum value is equal to $m_{\max}$. With (9.111) we then obtain

$$l_{\max} = l_1 + l_2 \tag{9.112}$$

In that l is an angular momentum quantum number, successive values of l differ from $l_{\max}$ in unit steps down to some minimum value. What is this minimum value? To obtain it, we note the following.

As noted previously, in the uncoupled representation there are $(2l_1 + 1)(2l_2 + 1)$ independent, common eigenstates of $\hat{L}_1{}^2$, $\hat{L}_2{}^2$, $\hat{L}_{1z}$, and $\hat{L}_{2z}$ relevant to the two-electron system. These states span a $(2l_1 + 1)(2l_2 + 1)$-dimensional space. A change in representation[1] from this basis to the common eigenstates of $\hat{L}^2$, $\hat{L}_z$, $\hat{L}_1{}^2$, and $\hat{L}_2{}^2$ maintains the dimensionality of this space. This observation affords a method of obtaining $l_{\min}$. That is, keep decreasing $l_{\max}$ in unit steps until the total number of independent states equals $(2l_1 + 1)(2l_2 + 1)$.

Now the number of independent eigenstates with a given l number is $2l + 1$. Then the value of $l_{\min}$ we seek satisfies the equation

$$\sum_{l=l_{\min}}^{l_1+l_2} (2l + 1) = (2l_1 + 1)(2l_2 + 1)$$

This relation is satisfied if we set

$$l_{\min} = |l_1 - l_2| \tag{9.113}$$

---

[1] The notion of changes in representation was discussed in Section 7.4 and will be developed further in Chapter 11.

In this manner we find that the values of l corresponding to a system comprised of two electrons with respective l values l_1 and l_2 are

$$l = |l_1 - l_2|, \ldots, l_1 + l_2 \tag{9.114}$$

For the problem cited above with one p electron ($l_1 = 1$) and one d electron ($l_2 = 2$), the total angular momentum may be any of the values

$$l = 1, 2, 3$$
$$L = \hbar\sqrt{2}, \qquad L = \hbar\sqrt{6}, \qquad L = \hbar\sqrt{12}$$

There are a totality of

$$N = (2 \times 1 + 1) + (2 \times 2 + 1) + (2 \times 3 + 1) = (2 \times 1 + 1)(2 \times 2 + 1) = 15$$

states, corresponding to these three values of l. For the case of two p electrons ($l_1 = l_2 = 1$) there are nine eigenstates. These are listed in Table 9.5.

The distinction between the coupled and uncoupled representations is brought out in the following two sets of eigenstate equations.

Coupled Representation

$$\begin{pmatrix} \hat{L}^2 \\ \hat{L}_z \\ \hat{L}_1{}^2 \\ \hat{L}_2{}^2 \end{pmatrix} |lml_1l_2\rangle = \hbar^2 \begin{pmatrix} l(l+1) \\ m/\hbar \\ l_1(l_1+1) \\ l_2(l_2+1) \end{pmatrix} |lml_1l_2\rangle$$

TABLE 9.5 Nine common eigenstates $|lml_1l_2\rangle$ of the opeators: $\hat{L}^2$, $\hat{L}_z$, $\hat{L}_1{}^2$, $\hat{L}_2{}^2$ for two p electrons

Diagramatic Representation[a]	$\lvert lml_1l_2\rangle$	$= \sum C_{m_1m_2} \lvert l_1m_1\rangle_1 \lvert l_2m_2\rangle_2$
$\uparrow\uparrow$	$\lvert 22\ 11\rangle$	$= \lvert 11\rangle_1 \lvert 11\rangle_2$
$\uparrow\cdot + \cdot\uparrow$	$\lvert 21\ 11\rangle$	$= \sqrt{\frac{1}{2}}\lvert 11\rangle_1\lvert 10\rangle_2 + \sqrt{\frac{1}{2}}\lvert 10\rangle_1\lvert 11\rangle_2$
$\uparrow\downarrow + \cdot\cdot + \downarrow\uparrow$	$\lvert 20\ 11\rangle$	$= \sqrt{\frac{1}{6}}\lvert 11\rangle_1\lvert 1,-1\rangle_2 + \sqrt{\frac{2}{3}}\lvert 10\rangle_1\lvert 10\rangle_2 + \sqrt{\frac{1}{6}}\lvert 1,-1\rangle_1\lvert 11\rangle_2$
$\cdot\downarrow + \downarrow\cdot$	$\lvert 2,-1\ 11\rangle$	$= \sqrt{\frac{1}{2}}\lvert 10\rangle_1\lvert 1,-1\rangle_2 + \sqrt{\frac{1}{2}}\lvert 1,-1\rangle_1\lvert 10\rangle_2$
$\downarrow\downarrow$	$\lvert 2,-2\ 11\rangle$	$= \lvert 1,-1\rangle_1\lvert 1,-1\rangle_2$
$\uparrow\cdot - \cdot\uparrow$	$\lvert 11\ 11\rangle$	$= \sqrt{\frac{1}{2}}\lvert 11\rangle_1\lvert 10\rangle_2 - \sqrt{\frac{1}{2}}\lvert 10\rangle_1\lvert 11\rangle_2$
$\uparrow\downarrow - \downarrow\uparrow$	$\lvert 10\ 11\rangle$	$= \sqrt{\frac{1}{2}}\lvert 11\rangle_1\lvert 1,-1\rangle_2 - \sqrt{\frac{1}{2}}\lvert 1,-1\rangle_2\lvert 11\rangle_2$
$\cdot\downarrow - \downarrow\cdot$	$\lvert 1.-1\ 11\rangle$	$= \sqrt{\frac{1}{2}}\lvert 10\rangle_1\lvert 1.-1\rangle_2 - \sqrt{\frac{1}{2}}\lvert 1,-1\rangle_1\lvert 10\rangle_2$
$\uparrow\downarrow - \cdot\cdot + \downarrow\uparrow$	$\lvert 00\ 11\rangle$	$= \sqrt{\frac{1}{3}}\lvert 11\rangle_1\lvert 1,-1\rangle_2 - \sqrt{\frac{1}{3}}\lvert 10\rangle_1\lvert 10\rangle_2 + \sqrt{\frac{1}{3}}\lvert 1,-1\rangle_1\lvert 11\rangle_2$

[a] The diagramatic representation of states is such that an up-arrow, a down-arrow, and a dot represent, respectively, $m = 1, -1$, and 0 of individual electrons.

Uncoupled Representation

$$\begin{pmatrix} \hat{L}_{1z} \\ \hat{L}_{2z} \\ \hat{L}_1{}^2 \\ \hat{L}_2{}^2 \end{pmatrix} |l_1 l_2 m_1 m_2\rangle = \hbar^2 \begin{pmatrix} m_1/\hbar \\ m_2/\hbar \\ l_1(l_1+1) \\ l_2(l_2+1) \end{pmatrix} |l_1 l_2 m_1 m_2\rangle$$

These equations are relevant, for example, to the case of two electrons, given that one is an l_1 electron and the other, an l_2 electron.

For three electrons, in the uncoupled representation the six operators

$$(\hat{L}_1{}^2, \hat{L}_{1z}, \hat{L}_2{}^2, \hat{L}_{2z}, \hat{L}_3{}^2, \hat{L}_{3z})$$

form a complete commuting set. Good quantum numbers associated with these states are $(l_1, m_1, l_2, m_2, l_3, m_3)$. In the more relevant coupled representation, the six operators

$$(\hat{L}^2, \hat{L}_z, \hat{L}_1{}^2, \hat{L}_2{}^2, \hat{L}_3{}^2, \hat{A}_1{}^2)$$

form a complete commuting set. The operator $\hat{A}_1{}^2$ is given by

$$\hat{A}_1{}^2 \equiv a_{12}(\hat{\mathbf{L}}_1 + \hat{\mathbf{L}}_2)^2 + a_{13}(\hat{\mathbf{L}}_1 + \hat{\mathbf{L}}_3)^2 + a_{23}(\hat{\mathbf{L}}_2 + \hat{\mathbf{L}}_3)^2 \tag{9.115}$$

where the a coefficients are arbitrary. If l' is the eigen-l-value related to $\hat{A}_1{}^2$, six good quantum numbers for the case at hand are $(l, m, l_1, l_2, l_3, l')$.

PROBLEMS

9.30 What are the eigenvalues of the set of operators $(\hat{L}_1{}^2, \hat{L}_{1z}, \hat{L}_2{}^2, \hat{L}_{2z})$ corresponding to the product eigenstate $|m_1 l_1\rangle |m_2 l_2\rangle$?

9.31 Let $\hat{\mathbf{J}}_1$ and $\hat{\mathbf{J}}_2$ be the respective angular momenta of the individual components of a two-component system. The total system has angular momentum $\hat{\mathbf{J}} = \hat{\mathbf{J}}_1 + \hat{\mathbf{J}}_2$. Show that:

(a) $\hat{\mathbf{J}}_1 \cdot \hat{\mathbf{J}}_2 = \frac{1}{2}(\hat{J}_{1+}\hat{J}_{2-} + \hat{J}_{1-}\hat{J}_{2+}) + \hat{J}_{1z}\hat{J}_{2z}$

(b) $\hat{J}^2 = \hat{J}_1{}^2 + \hat{J}_2{}^2 + 2\hat{J}_{1z}\hat{J}_{2z} + (\hat{J}_{1+}\hat{J}_{2-} + \hat{J}_{1-}\hat{J}_{2+})$

9.32 (a) Using the expansions developed in Problem 9.31, operate on the coupled angular momentum eigenstates for two p electrons as listed in Table 9.5 with $\hat{L}^2$ and $\hat{L}_z$, respectively, to verify the lm entries in each of the nine $|lml_1 l_2\rangle$ eigenstates.

(b) What are the Clebsch–Gordon coefficients involved in the expansion of the state $|0011\rangle$?

(c) What is the inner product $\langle 2011|0011\rangle$?

9.33 (a) With respect to the diagrammatic representation of states depicted in Table 9.5, what are the states corresponding to the diagrams

$$\psi_0 = \cdot\cdot, \qquad \psi_1 = \uparrow\downarrow + \downarrow\uparrow, \qquad \psi_3 = \uparrow\downarrow?$$

(b) Expand each of these functions in terms of the nine diagrams listed in Table 9.5.

(c) Are any of these three states eigenstates of $\hat{L}^2$? [*Hint*: Use the expansions obtained in part (b).]

(d) Two electrons are known to be in the coupled state ψ_1. What values of total angular momentum L will measurement find and with what probabilities will these values occur?

9.34 Two p electrons are in the state $|lml_1l_2\rangle = |1, -111\rangle$. If measurement is made of L_{1z} in this state, what values may be found and with what probability will these values occur?

9.35 Two p electrons are in the coupled angular momentum state $|lml_1l_2\rangle = |2,, -2, 11\rangle$. What is the joint probability of finding the two electrons with $L_{1z} = L_{2z} = -\hbar$?

9.36 How many independent eigenstates are there in the coupled representation for a two-component system, given that $l_1 = 5$ and $l_2 = 1$? Make a table listing the ml values for all these states.

9.37 Show that $\hat{A}_1{}^2$ as given by (9.115) commutes with $\hat{L}^2$ and $\hat{L}_z$.

9.38 The eigenstate corresponding to maximum l for the three-electron case is

$$|l, m, l_1, l_2, l_3, l'\rangle = |l_1, l_1\rangle |l_2, l_2\rangle |l_3, l_3\rangle$$

(a) What are the eigenvalues of $\hat{L}^2$, $\hat{L}_z$ corresponding to this state?

(b) What is the eigenvalue of the operator $\hat{A}_1{}^2$ given by (9.115) corresponding to this state?

9.5 TOTAL ANGULAR MOMENTUM FOR TWO OR MORE ELECTRONS

We are now concerned with the possible values the total angular momentum l numbers may assume for a system of N electrons with respective l_i values: $l_1, l_2, \ldots, l_N$, in the coupled representation. A totality of $(2l_1 + 1)(2l_2 + 1)\cdots(2l_N + 1)$ product states may be formed which are simultaneous eigenstates of the set of operators

$$(\hat{L}^2, \hat{L}_z{}^2, \hat{L}_1{}^2, \hat{L}_2{}^2, \ldots, \hat{L}_N{}^2)$$

We must make sure that our procedure for calculating these l values preserves this number of states. This affords a check that we have found all l values.

The possible values that l can assume may be obtained by one of two techniques. The first technique follows from the rule (9.114) for the addition of the angular momenta of two electrons with respective l values: l_1 and l_2. In this case the combined angular momentum

$$\hat{L}^2 = (\hat{\mathbf{L}}_1 + \hat{\mathbf{L}}_2)^2$$

has eigenvalues, $\hbar^2 l(l + 1)$, where

$$l = |l_1 + l_2|, \ldots, |l_1 - l_2|$$

Consider the case of three electrons. Their total angular momentum is given by

$$\hat{L}^2 = (\hat{\mathbf{L}}_1 + \hat{\mathbf{L}}_2 + \hat{\mathbf{L}}_3)^2$$

This may be rewritten in the form

$$\hat{L}^2 = (\hat{\mathbf{L}}' + \hat{\mathbf{L}}_3)^2$$
$$\hat{\mathbf{L}}' = \hat{\mathbf{L}}_1 + \hat{\mathbf{L}}_2$$

3 Suppose that one of the l values corresponding to $\hat{L}'^2$ is l'. Then the l values corresponding to the total angular momentum $\hat{L}^2$ are

$$l = |l' + l_3|, \ldots, |l' - l_3| \tag{9.116}$$

3. This again follows the rule of (9.114). For example, consider the case of three p electrons ($l_1 = l_2 = l_3 = 1$). Then for the first two electrons we have

$$l' = |l_1 + l_2|, \ldots, |l_1 - l_2| = 0, 1, 2$$

Adding the third electron gives [using (9.116)] the l values

$$\begin{array}{lcl} l' = 0, 1, 2 & & l = |l' + l_3|, \ldots, |l' - l_3| \\ l' = 0 & \longrightarrow & l = 1 \\ l' = 1 & \longrightarrow & l = 0, 1, 2 \\ l' = 2 & \longrightarrow & l = 1, 2, 3 \end{array}$$

4 Thus we obtain the result

$$\boxed{l = 0, 1, 2, 3 \qquad \text{for three } p \text{ electrons}}$$

There is a distinct eigenstate for each distinct manner in which l may be formed. This gives a total number of

$$(2 \times 0 + 1) + 3(2 \times 1 + 1) + 2(2 \times 2 + 1) + (2 \times 3 + 1)$$
$$= 1 + 9 + 10 + 7 = 27$$

states, which agrees with the product

$$(2l_1 + 1)(2l_2 + 1)(2l_3 + 1) = 3 \times 3 \times 3 = 27$$

-2 For the case of N electrons with respective l values $l_1, l_2, \ldots, l_N$, we follow a similar procedure. First, we add the angular momenta of the first two electrons. This gives

$$l' = |l_1 + l_2|, \ldots, |l_1 - l_2|$$

To these values we add the angular momentum of the third electron to obtain

$$l'' = |l' + l_3|, \ldots, |l' - l_3|$$

1 There is a separate sequence of l'' values for each value of l'. Adding the angular momentum of the fourth electron gives

$$l''' = |l'' + l_4|, \ldots, |l'' - l_4|$$

2 We continue in this manner until all individual angular momentum l values are accounted for. The final sequence gives all possible values of l. For three electrons the sequence of l'' gives all the values of l. For four electrons the sequence fór l''' gives the values of l.

1. **Addition Rules**

The values of total l obtained by sequential addition as described above may more simply be arrived at by the following rule. Consider N electrons with respective angular momentum values: $l_1, l_2, \ldots, l_N$. These values may always be ordered so that

$$l_1 \leq l_2 \leq \cdots \leq l_N$$

Let

$$\Lambda = \sum_{i=1}^{N-1} l_i$$

2 Then we have the following:

(a) If $l_N - \Lambda > 0$,

$$l^{\min} = l_N - \Lambda \tag{9.117}$$

(b) If $l_N - \Lambda \leq 0$,

$$l^{\min} = 0 \tag{9.118}$$

(c) In all cases

$$l^{\max} = \sum_{i=1}^{N} l_i \tag{9.119}$$

2. (d) The possible values of l that give the values of total L,

$$L^2 = (\mathbf{L}_1 + \mathbf{L}_2 + \cdots + \mathbf{L}_N)^2 = \hbar^2 l(l+1)$$

are given by

$$l = |l^{\max}|, |l^{\max} - 1|, \ldots, |l^{\min}| \tag{9.120}$$

As a simple example of this technique, consider the case of two p electrons and one f electron ($l_1 = l_2 = 1$, $l_3 = 3$). Then

$$\begin{aligned} \Lambda &= 1 + 1 = 2 \\ l_3 - \Lambda &= 3 - 2 = 1 = l^{\min} \\ l^{\max} &= 1 + 1 + 3 = 5 \end{aligned}$$

Therefore,

$l = 1, 2, 3, 4, 5$	for two p-electrons and one f-electron

The electron orbital angular momentum notation $s, p, d, f, \ldots$ stems from atomic physics. The correspondence between these letters and l values of individual electrons follows the scheme

symbol	s	p	d	f	g	h	$\ldots$
l value	0	1	2	3	4	5	$\ldots$

This notation will be used again in Chapter 12.

In Chapter 10 we will see how $\hat{L}^2$ enters the Hamiltonian for one and two-particle systems. The Y_l^m functions will take on further significance. They will emerge as the angular dependent factors of the energy eigenfunctions for these systems.

The topic of the addition of angular momentum is returned to in Chapter 11, where the rules developed above are applied to the addition of spin angular momentum. In Chapter 12 these rules are again applied to the addition of orbital and spin angular momentum as related to one- and two-electron atoms.

Mon. 27-7-1992
(21:00 GMT)
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Shirton Hotel

PROBLEMS

9.39 What are the possible values of l for:

(a) Four p electrons?

(b) Three p and one f ($l_4 = 3$) electrons?

9.40 What is the wavefunction (in Dirac notation) for three p electrons in the state with $l = m = 3$?

9.41 Show that the two schemes for obtaining the total l value for three electrons with respective l values l_1, l_2, and l_3, as described in the text, are equivalent.

9.42 (a) Show that the technique of sequential addition for obtaining total l values in the coupled representation gives

$$(2l_1 + l)(2l_2 + 1)\cdots(2l_N + 1)$$

eigenstates. (*Hint:* Assume that $l_1 < l_2 < \cdots < l_N$.)

(b) How many eigenstates are there for three f electrons?

9.43 In the uncoupled representation, N electrons are described by the simultaneous eigenstates of the $2N$ operators

$$(\hat{L}_1{}^2, \hat{L}_{1z}, \hat{L}_2{}^2, \hat{L}_{2z}, \ldots, \hat{L}_N{}^2, \hat{L}_{Nz})$$

In the coupled representation, the $N + 2$ commuting operators

$$(\hat{L}^2, \hat{L}_z, \hat{L}_1{}^2, \hat{L}_2{}^2, \ldots, \hat{L}_N{}^2)$$

are relevant, and there are $N + 2$ good quantum numbers corresponding to these operators. One suspects that $2N - (N + 2) = N - 2$ operators may be added to this sequence, yielding a set of $2N$ commuting operators.

(a) Construct such a set of $N - 2$ operators, $\{\hat{A}_i{}^2\}$.

(b) Show explicitly that the terms in the sum $\hat{A}_2{}^2$ commute with the sequence of $N + 2$ operators given above.

Answer (partial)

(a) The first operator is

$$\hat{A}_1{}^2 = a_{12}(\hat{\mathbf{L}}_1 + \hat{\mathbf{L}}_2)^2 + a_{13}(\hat{\mathbf{L}}_1 + \hat{\mathbf{L}}_3)^2 + \cdots = \sum_{i_1 \neq i_2}^{N} a_{i_1 i_2}(\hat{\mathbf{L}}_{i_1} + \hat{\mathbf{L}}_{i_2})^2$$

The second operator is

$$\hat{A}_2{}^2 = \sum_{i_1 \neq i_2 \neq i_3} a_{i_1 i_2 i_3}(\hat{\mathbf{L}}_{i_1} + \hat{\mathbf{L}}_{i_2} + \hat{\mathbf{L}}_{i_3})^2$$

The $(N - 2)$nd operator is

$$\hat{A}_{N-2}{}^2 = \sum_{i_1 \neq \cdots \neq i_{N-1}}^{N} a_{i_1 \cdots i_{N-1}}(\hat{\mathbf{L}}_{i_1} + \cdots \hat{\mathbf{L}}_{i_{N-1}})^2$$

9.44 The spherical harmonics $Y_l^m(\theta, \phi)$ are simultaneous eigenstates of $\hat{L}_z$ and $\hat{L}_2$. How must the Cartesian x, y, z axes be aligned with the spherical r, θ, ϕ frame in order for this to be true, or is the validity of this statement independent of the relative orientation of these two frames?

9.45 Suppose that L^2 is measured for a free particle and the value $6\hbar^2$ is found. If L_y is then measured, what possible values can result?

9.46 The parity operator, $\hat{\mathbb{P}}$, in three dimensions is defined by the equation $\hat{\mathbb{P}}f(r, \theta, \phi) = f(r, \pi - \theta, \pi + \phi)$. Show that $\hat{\mathbb{P}}Y_l^m = (-)^l Y_l^m$. That is, the parity of Y_l^m (odd or even) is the same as that of l. (Compare with Problem 6.23.)

The eigenfunction corresponding to the eigenenergy (10.75) is

$$f_n = A_n \mathscr{H}_n\left[\sqrt{\frac{m\Omega}{\hbar}}\,(y - y_0)\right] \exp\left[-\frac{1}{2}\sqrt{\frac{m\Omega}{\hbar}}\,(y - y_0)^2\right]$$

[recall (7.59)]. The nth-order Hermite polynomial is written $\mathscr{H}_n$, while A_n is a normalization constant. Together with (10.73), this form for f_n gives the wavefunction

(10.76)

$$\boxed{\varphi_n = A_n \mathscr{H}_n\left[\sqrt{\frac{m\Omega}{\hbar}}\,(y - y_0)\right] \exp\left[-\frac{1}{2}\sqrt{\frac{m\Omega}{\hbar}}\,(y - y_0)^2 + i(k_x x + k_z z)\right]}$$

for a charged particle moving in a uniform magnetic field which points in the z direction.

PROBLEMS

10.17 The following is a problem in classical physics. The force on a charged particle in a uniform magnetic field $\mathscr{B}$ is

$$\mathbf{F} = \frac{d}{dt}(m\mathbf{v}) = \frac{e}{c}\mathbf{v} \times \mathscr{B}$$

(a) Show that

$$\tfrac{1}{2}mv^2 = \text{constant}$$

with $\mathscr{B} = (0, 0, \mathscr{B})$.

(b) Show that

$$p_z = mv_z = \text{constant}$$

(c) Show that the motion of the particle is that of a helix whose axis is parallel to $\mathscr{B}$ and whose projection onto the xy plane is circular with constant angular frequency Ω.

(d) Show that the center of this circle in the xy plane has coordinates

$$y_0 = \frac{-cp_x}{e\mathscr{B}} = \frac{-cmv_x}{e\mathscr{B}} + y$$

$$x_0 = \frac{cmv_y}{e\mathscr{B}} + x = \frac{cp_y}{e\mathscr{B}} + x$$

Note that p_x, canonical momentum, is not equal to mv_x for $A = (A_x, 0, 0)$. The correct relation follows from (1.14) and (10.71).

10.18 Show that the operator

$$\hat{x}_0 \equiv \hat{x} + \frac{c\hat{p}_y}{e\mathscr{B}}$$

commutes with $\hat{H}$ as given in (10.72) but does not commute with

$$\hat{y}_0 = \frac{-c\hat{p}_x}{e\mathscr{B}}$$

These operators correspond to the coordinates of the center of the related projected classical motion in the xy plane. In quantum mechanics we see that although x_0 and E, or y_0 and E, may, respectively, be specified simultaneously, x_0 and y_0 may not be simultaneously specified.

10.19 (a) What is the vector potential **A** which gives the uniform $\mathscr{B}$ field $(0, 0, \mathscr{B})$ which includes $A_x = A_z = 0$?

(b) What is the form of the wavefunctions φ_n corresponding to this choice of vector potential? How do they compare to the wavefunctions corresponding to $A_y = A_z = 0$ found in the text?

(c) How do the eigenenergies compare to those found in the representation $A_y = A_z = 0$?

10.20 What is the nature of the frequency spectrum emitted by a charged particle moving in a uniform magnetic field? (Assume that the kinetic energy parallel to $\mathscr{B}$ does not change.) For an electron moving in a $\mathscr{B}$ field of 10^4 gauss, what type of radiation is this (x rays, microwaves, etc.)?

10.5 THE TWO-PARTICLE PROBLEM

Coordinates Relative to the Center of Mass

When dealing with systems containing more than one particle (e.g., an atom), it is convenient to separate the motion into that of the center of mass of the system and motion relative to the center of mass. This separation is effected through a partitioning of the Hamiltonian into a part, H_{CM}, involving center of mass coordinates, and a part, H_{rel}, containing coordinates relative to the center of mass.

For example, consider the two-particle Hamiltonian

$$H = \frac{{p_1}^2}{2m_1} + \frac{{p_2}^2}{2m_2} + V(|\mathbf{r}_1 - \mathbf{r}_2|) \tag{10.77}$$

The potential of interaction $V(|\mathbf{r}_1 - \mathbf{r}_2|)$ is a function only of the radial distance between the particles. For instance, for the hydrogen atom, the interaction V is the Coulomb potential

$$V = -\frac{e^2}{r} \tag{10.78}$$

where we have written r for the distance between particles, $|\mathbf{r}_1 - \mathbf{r}_2|$. Such potentials, which are only a function of the scalar distance r, are called *central potentials.*

In the Hamiltonian above, $\mathbf{p}_1$ and $\mathbf{p}_2$ are the linear momenta of particle 1 and particle 2, respectively, while m_1 and m_2 are the respective masses of these particles.

A two-particle system has six degrees of freedom. These are characterized by the parameters $(\mathbf{r}_1, \mathbf{p}_1; \mathbf{r}_2, \mathbf{p}_2)$. The partitioning of the Hamiltonian into $H_{\mathrm{CM}} + H_{\mathrm{rel}}$ is generated through the transformation of variables

$$(\mathbf{r}_1, \mathbf{p}_1; \mathbf{r}_2, \mathbf{p}_2) \to (\mathbf{r}, \mathbf{p}; \mathscr{R}, \mathscr{P}) \tag{10.79}$$

where

$$\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2, \qquad \mathscr{P} = \mathbf{p}_1 + \mathbf{p}_2$$

$$\mathbf{p} = \frac{m_2\mathbf{p}_1 - m_1\mathbf{p}_2}{m_1 + m_2}, \qquad \mathscr{R} = \frac{m_1\mathbf{r}_1 + m_2\mathbf{r}_2}{m_1 + m_2} \tag{10.80}$$

Using these equations the Hamiltonian (10.77) is transformed to the sum

$$H = \frac{\mathscr{P}^2}{2M} + \left[\frac{p^2}{2\mu} + V(r)\right] \equiv H_{\mathrm{CM}} + H_{\mathrm{rel}} \tag{10.81}$$

where the reduced mass μ and the total mass M are

$$\mu = \frac{m_1 m_2}{m_1 + m_2}, \qquad M = m_1 + m_2 \tag{10.82}$$

Equation (10.81) represents the desired separation of H into the Hamiltonian of the center of mass, H_{CM}, and the Hamiltonian of the coordinates relative to the center of mass, H_{rel} (Fig. 10.8). Since $\mathscr{R}$ is absent in H (i.e., $\mathscr{R}$ is a cyclic coordinate;

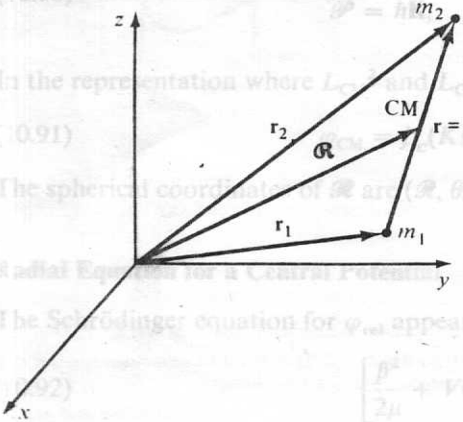

FIGURE 10.8 The relative vector r and the center-of-mass vector $\mathscr{R}$. In the classical motion, $\mathscr{P} = M\dot{\mathscr{R}}$ = constant = $\mathscr{P}(0)$ = the initial value of $\mathscr{P}(t)$. At any time t

$$\mathscr{R}(t) = \mathscr{R}(0) + \frac{\mathscr{P}(0)t}{M}$$

Solving the dynamical equations (viz., Hamilton's equations) using H_{rel} gives $\mathbf{r}(t)$, which when affixed to $\mathscr{R}(t)$ gives the motion in the "lab frame."

see Section 1.2), the momentum of the center of mass, $\mathscr{P}$, is constant. The center of mass moves in straight-rectilinear motion, characteristic of a free particle of mass M. The motion relative to the center of mass is that of a particle of mass μ moving in the central potential $V(r)$.

The Transformation of $\hat{H}$

For the quantum mechanical case, the transformation of $\hat{H}$ is again effected with the equations (10.80), which are now interpreted as operator relations. Cartesian components of "old" coordinate and momentum operators $(\hat{\mathbf{r}}_1, \hat{\mathbf{p}}_1; \hat{\mathbf{r}}_2, \hat{\mathbf{p}}_2)$ obey the commutation relations

$$\left.\begin{aligned}[][\hat{r}_{1j}, \hat{p}_{1j}] &= i\hbar \\ [\hat{r}_{2j}, \hat{p}_{2j}] &= i\hbar\end{aligned}\right\} \quad j = 1, 2, 3 \tag{10.83}$$

These are the only nonvanishing commutators. With these relations and (10.80), one obtains that the only nonvanishing commutator relations for components of the "new" operators $(\hat{\mathbf{r}}, \hat{\mathbf{p}}; \hat{\mathscr{R}}, \hat{\mathscr{P}})$ are

$$\left.\begin{aligned}[][\hat{r}_j, \hat{p}_j] &= i\hbar \\ [\hat{\mathscr{R}}_j, \hat{\mathscr{P}}_j] &= i\hbar\end{aligned}\right\} \quad j = 1, 2, 3 \tag{10.84}$$

Thus, in obtaining

$$\begin{gathered}\hat{H} = \hat{H}_{\text{CM}} + \hat{H}_{\text{rel}} \\ \hat{H}_{\text{CM}} = \frac{\hat{\mathscr{P}}^2}{2M} \\ \hat{H}_{\text{rel}} = \frac{\hat{p}^2}{2\mu} + V(r)\end{gathered} \tag{10.85}$$

the Hamiltonian is separated into two components involving coordinates that are independent of one another. For such cases, the Schrödinger equation has product eigenfunctions

$$\bar{\varphi} = \varphi_{\text{CM}}(\mathscr{R})\varphi_{\text{rel}}(\mathbf{r}) \tag{10.86}$$

and summational eigenvalues

$$\bar{E} = E_{\text{CM}} + E_{\text{rel}} \tag{10.87}$$

where

$$\begin{gathered}\hat{H}\bar{\varphi} = \bar{E}\bar{\varphi} \\ \hat{H}_{\text{CM}}\varphi_{\text{CM}} = E_{\text{CM}}\varphi_{\text{CM}} \\ \hat{H}_{\text{rel}}\varphi_{\text{rel}} = E_{\text{rel}}\varphi_{\text{rel}}\end{gathered} \tag{10.88}$$

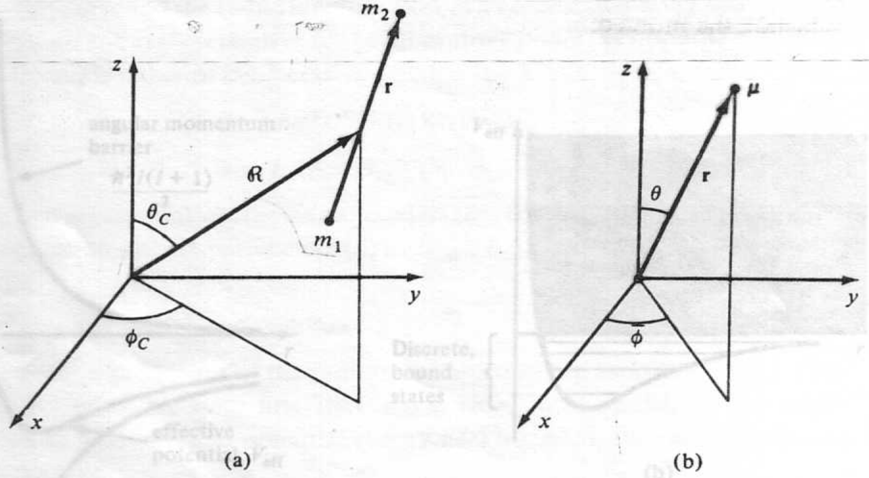

FIGURE 10.9 (a) Spherical angle variables for the center-of-mass radius vector $\mathscr{R}$. (b) Coordinates relative to the center of mass.

The Schrödinger equation for the center of mass appears explicitly as

$$\frac{\hat{\mathscr{P}}^2}{2M}\varphi_{\mathrm{CM}} = E_{\mathrm{CM}}\varphi_{\mathrm{CM}} \tag{10.89}$$

This is the Schrödinger equation for a free particle of mass M. Its solution was obtained in the previous section. With the linear momentum $\mathscr{P}$ specified, the states are

$$\begin{gathered}\varphi_{\mathrm{CM}} = Ae^{i\mathbf{K}\cdot\mathscr{R}} \\ \mathscr{P} = \hbar\mathbf{K}, \qquad E_{\mathrm{CM}} = \frac{\hbar^2K^2}{2M}\end{gathered} \tag{10.90}$$

In the representation where ${L_{\mathrm{CM}}}^2$ and L_{CM_z} are specified, the eigenstates are

$$\varphi_{\mathrm{CM}} = j_{l_C}(K\mathscr{R})Y_{l_C}{}^{m_C}(\theta_C, \phi_C) \tag{10.91}$$

The spherical coordinates of $\mathscr{R}$ are $(\mathscr{R}, \theta_C, \phi_C)$ (see Fig. 10.9a).

Radial Equation for a Central Potential

The Schrödinger equation for φ_{rel} appears as (dropping the "rel" subscript)

$$\left[\frac{\hat{p}^2}{2\mu} + V(r)\right]\varphi = E\varphi \tag{10.92}$$

For central potential functions $V(r)$, it proves most convenient to express the above Hamiltonian in spherical coordinates. The interparticle radius $\mathbf{r}$ has coordinates (r, θ, ϕ) with the polar axis depicted as lying in the z direction (see Figure 10.9b).

In these coordinates the Schrödinger equation above becomes

$$\hat{H}\varphi = \left[\frac{\hat{p}_r{}^2}{2\mu} + \frac{\hat{L}^2}{2\mu r^2} + V(r)\right]\varphi = E\varphi \tag{10.93}$$

First, we note that $\hat{L}^2$ and $\hat{L}_z$ both commute with $\hat{H}$. The remaining components in $\hat{H}$ are all isotropic forms and are therefore unaffected by angular momentum operators. It follows that $\hat{H}$, $\hat{L}^2$, and $\hat{L}_z$ have simultaneous eigenstates. These are given by the product form

$$\varphi = R(r)Y_l^m(\theta, \phi) \tag{10.94}$$

Substituting this solution into the Schrödinger equation above gives the "radial" equation

$$\left[\frac{\hat{p}_r{}^2}{2\mu} + \frac{\hbar^2 l(l+1)}{2\mu r^2} + V(r)\right]R(r) = ER(r) \tag{10.95}$$

This is an ordinary, second-order, linear differential equation for the radial dependent component of the wavefunction $R(r)$. Since only one variable is involved in (10.95), it is suggestive of one-dimensional motion with the effective potential

$$V_{\text{eff}} = V(r) + \frac{\hbar^2 l(l+1)}{2\mu r^2} \tag{10.96}$$

The second term in this expression is called the "angular momentum barrier." It becomes infinitely high as $r \to 0$ and acts as a repulsive core, which for $l > 0$ prevents collapse of the system (see Fig. 10.10).

The normalization of the eigenstates (10.94) is given by the integral

$$\begin{aligned} \langle RY_l^m | RY_l^m \rangle &= \int_0^\infty dr\, r^2 \int_{4\pi} d\Omega\, |R(r)Y_l^m(\theta, \phi)|^2 = 1 \\ &= \int_0^\infty r^2 |R(r)|^2\, dr = 1 \end{aligned} \tag{10.97}$$

The radial displacement r separates the two particles m_1 and m_2. If we envision particle m_1 at the origin, then

$$Pr^2\, dr\, d\Omega = |R(r)Y_l^m(\theta, \phi)|^2 r^2\, dr\, d\Omega \tag{10.98}$$

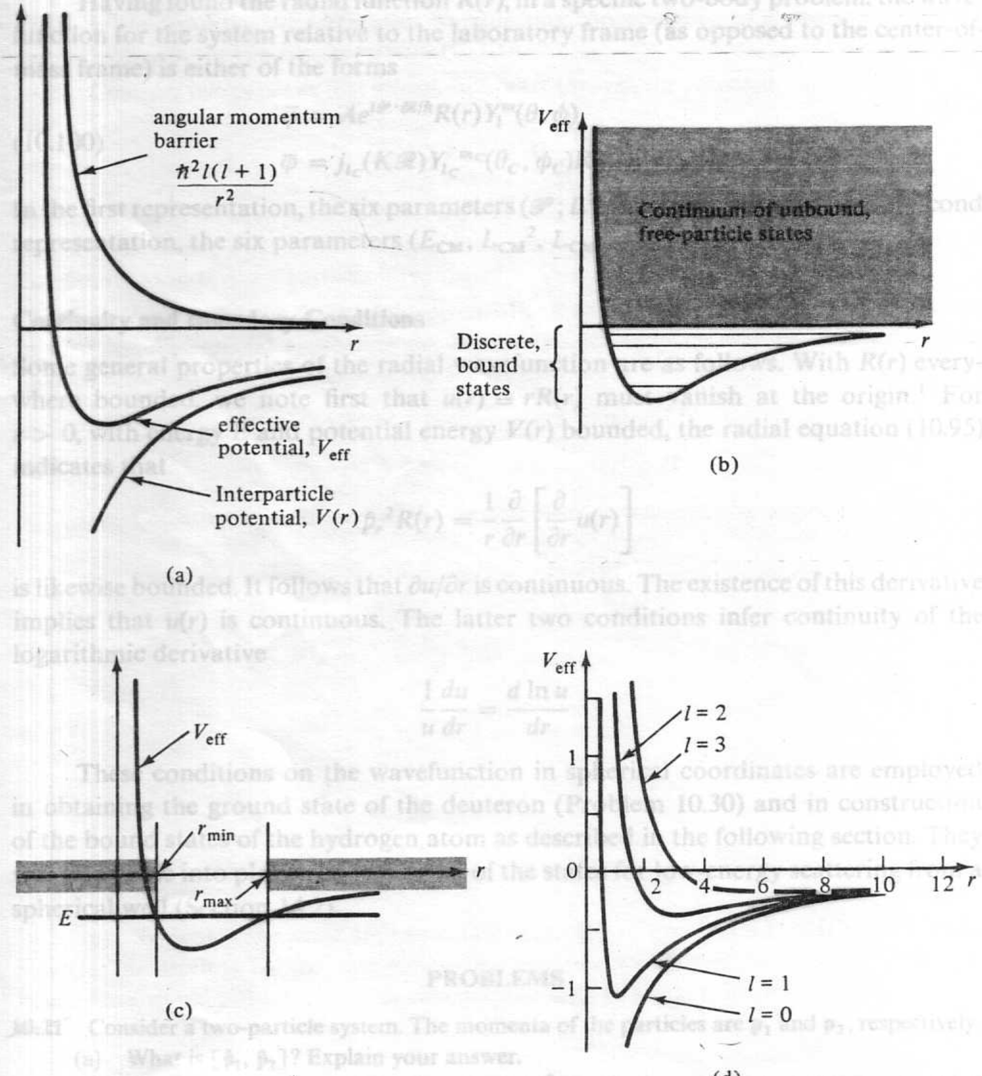

FIGURE 10.10 **(a) The effective potential in relation to the angular momentum barrier**

$$V_{\text{eff}} = V(r) + \frac{\hbar^2 l(l+1)}{r^2}$$

(b) Nature of the quantum mechanical energy spectrum for central potential problems. (c) The classical motion corresponding to the energy E. Shaded regions define classically forbidden domains. (d) The effective potential energy V_{eff} for hydrogen for several values of the orbital quantum number l. Units of r are angstroms. V_{eff} is in units of 10^{-11} erg.

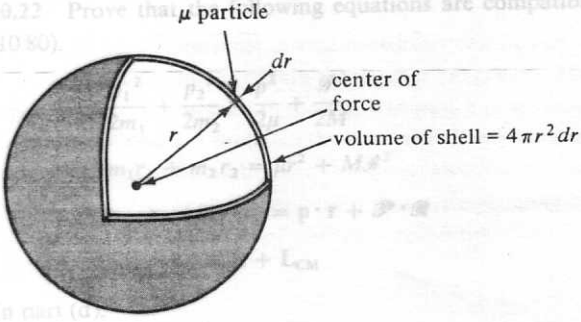

FIGURE 10.11 Probability of finding the fictitious μ particle in a spherical shell between r and $r + dr$ is

$$P_r\,dr = |R(r)r|^2\,dr$$

This is also the probability of finding m_2 in a spherical shell about m_1 in the configuration shown (or m_1 in a shell about m_2).

is the probability of finding m_2 in the *volume element* $r^2\,dr\,d\Omega$ about m_1 (an equally valid statement is obtained with m_1 and m_2 reversed). What is the probability of finding m_2 in a *spherical shell* of radius between r and $r + dr$, about m_1? The answer is (Fig. 10.11)

$$P_r\,dr = \left(\int_{4\pi} Pr^2\,d\Omega\right) dr = |R(r)|^2 r^2\,dr \equiv |u(r)|^2\,dr \tag{10.99}$$

so that

$$\int_0^\infty |u(r)|^2\,dr = 1$$

The classically forbidden domains (see Chapter 1) correspond to values of r for which $E < V$. The related property for a spherical quantum mechanical system is that the probability density $|u(r)|^2$ becomes small in these domains (see Figs. 10.10c and 10.12).

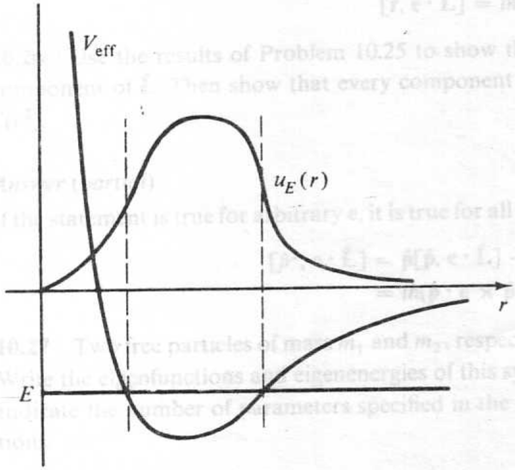

FIGURE 10.12 The radial probability amplitude u_E corresponding to the energy E decays to zero in the classically forbidden domain.

Having found the radial function $R(r)$, in a specific two-body problem, the wavefunction for the system relative to the laboratory frame (as opposed to the center-of-mass frame) is either of the forms

$$\begin{aligned} \bar{\varphi} &= Ae^{i\mathscr{P}\cdot\mathscr{R}/\hbar}R(r)Y_l^m(\theta,\phi) \\ \bar{\varphi} &= j_{l_C}(K\mathscr{R})Y_{l_C}{}^{m_C}(\theta_C,\phi_C)R(r)Y_l^m(\theta,\phi) \end{aligned} \tag{10.100}$$

In the first representation, the six parameters $(\mathscr{P}; L^2, L_z, E)$ are specified. In the second representation, the six parameters $(E_{\mathrm{CM}}, L_{\mathrm{CM}}{}^2, L_{\mathrm{CM}_z}; L^2, L_z, E)$ are specified.

Continuity and Boundary Conditions

Some general properties of the radial wavefunction are as follows. With $R(r)$ everywhere bounded, we note first that $u(r) \equiv rR(r)$ must vanish at the origin.[1] For $r > 0$, with energy E and potential energy $V(r)$ bounded, the radial equation (10.95) indicates that

$$\hat{p}_r{}^2 R(r) = \frac{1}{r}\frac{\partial}{\partial r}\left[\frac{\partial}{\partial r}u(r)\right]$$

is likewise bounded. It follows that $\partial u/\partial r$ is continuous. The existence of this derivative implies that $u(r)$ is continuous. The latter two conditions infer continuity of the logarithmic derivative

$$\frac{1}{u}\frac{du}{dr} = \frac{d\ln u}{dr}$$

These conditions on the wavefunction in spherical coordinates are employed in obtaining the ground state of the deuteron (Problem 10.30) and in construction of the bound states of the hydrogen atom as described in the following section. They will also come into play in construction of the states for low-energy scattering from a spherical well (Section 14.2).

PROBLEMS

10.21 Consider a two-particle system. The momenta of the particles are $\mathbf{p}_1$ and $\mathbf{p}_2$, respectively.

(a) What is $[\hat{\mathbf{p}}_1, \hat{\mathbf{p}}_2]$? Explain your answer.

(b) Use the answer to part (a) to show that $[\hat{\mathbf{p}}, \hat{\mathscr{P}}] = 0$, where $\mathbf{p}$ is the "relative" momentum [defined in (10.80)] and $\mathscr{P}$ is the momentum of the center of mass.

(c) The particles interact under a potential that is a function of the distance between them. As shown in the text, transformation to coordinates relative to the center of mass effects a partitioning of the Hamiltonian, $\hat{H} = \hat{H}_{\mathrm{CM}} + \hat{H}_{\mathrm{rel}}$. What is $[\hat{H}_{\mathrm{CM}}, \hat{H}_{\mathrm{rel}}]$?

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[1] Dirac obtains this boundary condition from the stipulation that solutions to the Schrödinger equation in spherical coordinates agree with those obtained in Cartesian coordinates. For further discussion, see P. A. M. Dirac, *The Principles of Quantum Mechanics*, 4th ed., Oxford University Press, New York, 1958.

10.22 Prove that the following equations are compatible with the transformation equations (10.80).

(a) $\dfrac{p_1{}^2}{2m_1}+\dfrac{p_2{}^2}{2m_2}=\dfrac{p^2}{2\mu}+\dfrac{\mathscr{P}^2}{2M}$

(b) $m_1r_1+m_2r_2=\mu r^2+M\mathscr{R}^2$

(c) $\mathbf{p}_1\cdot\mathbf{r}_1+\mathbf{p}_2\cdot\mathbf{r}_2=\mathbf{p}\cdot\mathbf{r}+\mathscr{P}\cdot\mathscr{R}$

(d) $\mathbf{L}_1+\mathbf{L}_2=\mathbf{L}+\mathbf{L}_{\mathrm{CM}}$

In part (d),

$$\mathbf{L}_1=\mathbf{r}_1\times\mathbf{p}_1 \qquad \mathbf{L}=\mathbf{r}\times\mathbf{p}$$
$$\mathbf{L}_2=\mathbf{r}_2\times\mathbf{p}_2 \qquad \mathbf{L}_{\mathrm{CM}}=\mathscr{R}\times\mathscr{P}$$

10.23 At a particular time, the wavefunction of a mass m moving in a three-dimensional potential well is

$$\varphi=A(x+y+z)e^{-k_0r}$$

(a) Calculate the normalization constant A.

(b) What is the probability that measurement of L^2 and L_z finds $2\hbar^2$ and 0, respectively? (See Table 9.1.)

(c) What is the probability of finding the particle in the sphere $r\le k_0{}^{-1}$?

10.24 For a two-particle system (m_1, m_2), what is the fractional distance to the center of mass from m_1 and m_2, respectively? What are these numbers for hydrogen?

10.25 Let **e** be a unit vector in an arbitrary but fixed direction. Show that the commutators between the components of $\hat{\mathbf{r}}$ and $\hat{\mathbf{p}}$, respectively, with the component $\mathbf{e}\cdot\hat{\mathbf{L}}$ obey the relations

$$[\hat{\mathbf{p}},\mathbf{e}\cdot\hat{\mathbf{L}}]=i\hbar\mathbf{e}\times\hat{\mathbf{p}}$$
$$[\hat{\mathbf{r}},\mathbf{e}\cdot\hat{\mathbf{L}}]=i\hbar\mathbf{e}\times\hat{\mathbf{r}}$$

10.26 Use the results of Problem 10.25 to show that $\hat{p}^2$, $\hat{r}^2$, and $\hat{\mathbf{r}}\cdot\hat{\mathbf{p}}$ all commute with every component of $\hat{\mathbf{L}}$. Then show that every component of $\hat{\mathbf{L}}$ commutes with any isotropic function $f(r^2)$.

Answer (*partial*)

If the statement is true for arbitrary **e**, it is true for all components of $\hat{\mathbf{L}}$.

$$\begin{aligned}[\hat{p}^2,\mathbf{e}\cdot\hat{\mathbf{L}}]&=\hat{\mathbf{p}}[\hat{\mathbf{p}},\mathbf{e}\cdot\hat{\mathbf{L}}]+[\hat{\mathbf{p}},\mathbf{e}\cdot\hat{\mathbf{L}}]\cdot\hat{\mathbf{p}}\\&=i\hbar(\hat{\mathbf{p}}\cdot\mathbf{e}\times\hat{\mathbf{p}}+\mathbf{e}\times\hat{\mathbf{p}}\cdot\hat{\mathbf{p}})=0\end{aligned}$$

10.27 Two free particles of mass m_1 and m_2, respectively, move in 3-space. They do not interact. Write the eigenfunctions and eigenenergies of this system in as many representations as you can. Indicate the number of parameters specified in the eigenstates associated with these representations.

10.28 Write down the time-dependent wavefunction corresponding to eigenstates for a two-particle system in the two representations (10.100).

10.29 Consider two particles that attract each other through the potential

$$V(r) = -\frac{\hbar^2 K^2}{2\mu r^2}$$

The displacement between particles is r, K is a constant, and μ is reduced mass. In states of definite angular momentum, what are the values of the angular momentum quantum number l for which the effective force between particles is repulsive?

10.30 In Problem 8.1 the depth of the potential well appropriate to a deuteron was evaluated using a one-dimensional approximation. A more refined estimate may be obtained using a three-dimensional spherical well with characteristics

$$\begin{aligned} V(r) &= -|V|, & r < a \quad &\text{region I} \\ V(r) &= 0 & r \geq a \quad &\text{region II} \end{aligned}$$

(a) Construct components of the ground-state wavefunction in regions I and II, respectively.

(b) Show that matching conditions at $r = a$ give the dispersion relation

$$\eta = -\xi \cot \xi$$

$$\rho^2 = \xi^2 + \eta^2$$

where

$$\rho^2 \equiv \frac{2m|V|a^2}{\hbar^2}, \qquad \xi \equiv ka, \quad \eta \equiv \kappa a$$

$$|E| = \frac{\hbar^2 \kappa^2}{2m}, \qquad |V| - |E| = \frac{\hbar^2 k^2}{2m}$$

(c) To within the same approximation suggested in Problem 8.1, obtain a numerical value for the depth $|V|$ of the three-dimensional deuteron well. From the ratio $|E|/|V|$ for this bound state, would you say that the deuteron is a strongly or a weakly bound nucleus?

Answers (partial)

(a) Component wavefunctions in the well domain, region I, are the spherical Bessel functions. The ground-state component is therefore

$$\varphi_{\text{I}} = \frac{\sin kr}{kr}$$

In region II the component ground-state wavefunction is exponentially damped.

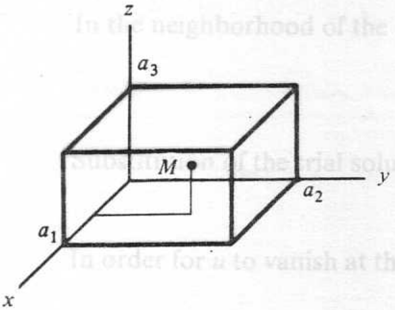
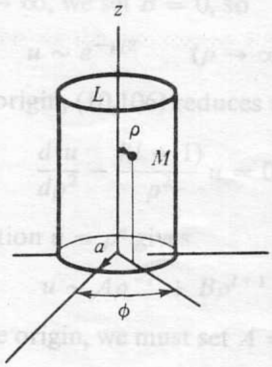
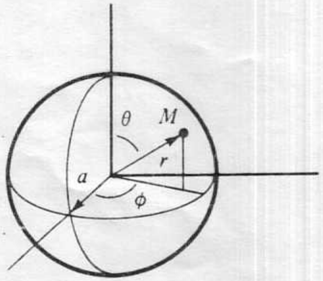
$$\varphi_{\text{II}} = A\,\frac{e^{-\kappa r}}{\kappa r}$$

(b) Here one must invoke continuity of $d \ln u/dr$.

(c) You should obtain the answer $|E|/|V| = 0.08$. This value implies that the binding energy is small compared to the depth of well, and we may conclude that the proton and neutron are weakly bound. A sketch of the normalized wavefunction further reveals that there is approximately only one chance in three that the nucleons are closer together than the well radius a.

10.31 Show by explicit calculation that the eigenfunctions and eigenenergies as given in Table 10.2 are correct for each of the three respective "box" configurations shown. (Primes denote differentiation.)

TABLE 10.2 Solutions to the three fundamental box problems in quantum mechanics

The Rectangular Box	The Cylindrical Box	The Spherical Box
Edge Lengths a_1, a_2, a_3	Radius a, Height b	Radius a
		
Hamiltonian		
$\hat{H} = (\hat{p}_x{}^2 + \hat{p}_y{}^2 + \hat{p}_z{}^2)/2M$	$\hat{H} = (\hat{p}_\rho{}^2 + \hat{p}_z{}^2 + \hat{L}_z{}^2\ \rho^2)/2M$	$\hat{H} = (\hat{p}_r{}^2 + \hat{L}^2/r^2)/2M$
$\hat{p}_x{}^2 = \left(-i\hbar \dfrac{\partial}{\partial x}\right)^2$	$\hat{p}_\rho{}^2 = -\hbar^2 \dfrac{1}{\rho}\dfrac{\partial}{\partial\rho}\left(\rho\dfrac{\partial}{\partial\rho}\right)$	$\hat{p}_r{}^2 = -\hbar^2\left(\dfrac{1}{r}\dfrac{\partial}{\partial r} r\right)^2$
Eigenfunction		
$\varphi_{qst} = A_{qst} \sin k_q x \sin k_s y \sin k_t z$	$\varphi_{qmn} = A_{qmn} J_m(K_{mn}\rho) \sin k_q z e^{im\phi}$	$\varphi_{nlm} = A_{nlm} j_l(k_{ln}r) Y_l{}^m(\theta, \phi)$
$(A_{qst})^2 = 8/a_1 a_2 a_3$	$(A_{qmn})^2 = 2/\pi b[aJ_m'(K_{mn}a)]^2$	$(A_{nlm})^2 = 2/k_{ln}[a^2 j_l'(k_{ln}a)]^2$
$\sin k_q a_1 = \sin k_s a_2 = \sin k_t a_3 = 0$	$\sin k_q b = J_m(K_{mn}a) = 0$	$j_l(k_{ln}a) = 0$
Wave Equation	*Bessel's Equation*	*Spherical Bessel Equation*
$\left(\dfrac{d^2}{dx^2} + k^2\right) \sin kx = 0$	$\left[\dfrac{1}{x^2}\left(x\dfrac{d}{dx}\right)^2 + 1 - \dfrac{m^2}{x^2}\right] J_m(x) = 0$	$\left[\left(\dfrac{1}{x}\dfrac{d}{dx}x\right)^2 + 1 - \dfrac{l(l+1)}{x^2}\right] j_l(x) = 0$
Eigenenergy		
$E_{qst} = \hbar^2(k_q{}^2 + k_s{}^2 + k_t{}^2)/2M$	$E_{qmn} = \hbar^2(K_{mn}{}^2 + k_q{}^2)\ 2M$	$E_{nl} = \hbar^2 k_{ln}{}^2/2M$

10.6 THE HYDROGEN ATOM

Hamiltonian and Eigenenergies

The (relative) Hamiltonian for the hydrogen atom (more accurately, for a "hydrogenic" atom[1] of atomic number Z) appears as

$$\hat{H} = \frac{\hat{p}_r^{\,2}}{2\mu} + \frac{\hat{L}^2}{2\mu r^2} - \frac{Ze^2}{r} \tag{10.101}$$

The corresponding Schrödinger equation is

$$\left(\frac{\hat{p}_r^{\,2}}{2\mu} + \frac{\hat{L}^2}{2\mu r^2} - \frac{Ze^2}{r}\right)\varphi = E\varphi = -|E|\varphi \tag{10.102}$$

We are seeking the *bound states* of hydrogen. These correspond to the negative eigenenergies, $E = -|E|$. Setting $\varphi = R(r)Y_l^m(\theta, \phi)$ in the latter equation gives the radial equation (10.95)

$$\left[\frac{-\hbar^2}{2\mu}\left(\frac{1}{r}\frac{d^2}{dr^2}r\right) + \frac{\hbar^2 l(l+1)}{2\mu r^2} - \frac{Ze^2}{r} + |E|\right]R = 0 \tag{10.103}$$

Changing the dependent variable to

$$u = rR$$

introduced previously in (10.99), gives

$$\left(-\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2} - \frac{2\mu Ze^2}{\hbar^2 r} + \frac{2\mu|E|}{\hbar^2}\right)u = 0 \tag{10.104}$$

Introducing the notation

$$\rho \equiv 2\kappa r, \qquad \frac{\hbar^2\kappa^2}{2\mu} = |E|$$

$$\lambda^2 = \left(\frac{Z}{\kappa a_0}\right)^2 = \frac{Z^2\mathbb{R}}{|E|} \tag{10.105}$$

$$\mathbb{R} = \frac{\hbar^2}{2\mu a_0^{\,2}}, \qquad a_0 = \frac{\hbar^2}{\mu e^2}$$

---

[1] Hydrogenic atoms are atoms that are ionized with all but one electron bound to the nucleus which carries the charge $+Ze$ (e.g., He^+, Li^{++}, etc.).

where $\mathbb{R}$ is the Rydberg constant[1] (2.13) and a_0 is the Bohr radius (2.14), the radial equation may be further simplified to the form

$$\frac{d^2u}{d\rho^2} - \frac{l(l+1)}{\rho^2}u + \left(\frac{\lambda}{\rho} - \frac{1}{4}\right)u = 0 \tag{10.106}$$

For large values of ρ this equation reduces to

$$\frac{d^2u}{d\rho^2} - \frac{u}{4} = 0$$

so that

$$u \sim Ae^{-\rho/2} + Be^{\rho/2}$$

In order that u vanish as $\rho \to \infty$, we set $B = 0$, so

$$u \sim e^{-\rho/2} \qquad (\rho \to \infty)$$

In the neighborhood of the origin, (10.106) reduces to

$$\frac{d^2u}{d\rho^2} - \frac{l(l+1)}{\rho^2}u = 0$$

Substitution of the trial solution $u = \rho^q$ gives

$$u \sim A\rho^{-l} + B\rho^{l+1}$$

In order for u to vanish at the origin, we must set $A = 0$. This gives

$$u \sim \rho^{l+1} \qquad (\rho \to 0)$$

With these two asymptotic forms at hand, we are prepared to solve (10.106) through a polynomial expansion. Solution in the form

$$u(\rho) = e^{-\rho/2}\rho^{l+1}F(\rho)$$

$$F(\rho) = \sum_{i=0}^{\infty} C_i\rho^i \tag{10.107}$$

with F finite everywhere, gives the proper behavior at $\rho \sim 0$ and $\rho \sim \infty$. Substituting (10.107) for u into (10.106), we obtain

$$\left[\rho\frac{d^2}{d\rho^2} + (2l + 2 - \rho)\frac{d}{d\rho} - (l + 1 - \lambda)\right]F(\rho) = 0 \tag{10.108}$$

Note that for a given value of the orbital quantum number l, this is an eigenvalue equation with eigenvalue λ. The values of λ (or, equivalently, the eigenenergies,

---

[1] The Rydberg constant written with m in place of μ (i.e., assuming infinite proton mass) is sometimes written $\mathbb{R}_\infty$.

$|E|$) are those values which ensure that $F(\rho)$ is finite for all ρ. Substituting the series (10.107) into the latter equation and equating coefficients of equal powers in ρ gives the *recurrence relation*

$$C_{i+1} = \frac{(i+l+1)-\lambda}{(i+1)(i+2l+2)} C_i \equiv \Gamma_{il} C_i \tag{10.109}$$

In the limit that $i \to \infty$, this relation becomes

$$C_{i+1} \sim \frac{C_i}{i}$$

which is the same ratio of coefficients obtained in the expansion

$$e^{\rho} = \sum C_i \rho^i = \sum \frac{\rho^i}{i!}$$

$$\frac{C_{i+1}}{C_i} = \frac{i!}{(i+1)!} = \frac{1}{i+1} \sim \frac{1}{i}$$

It follows that the form of $u(\rho)$ generated by the series (10.107) behaves as

$$u(\rho) \sim e^{-\rho/2} \rho^{l+1} e^{\rho} = e^{\rho/2} \rho^{l+1}$$

which diverges for large ρ. To obtain a finite wavefunction, the expansion (10.107) for any given value of l must terminate at some finite value of i, which we will call $i_{\max}$. At this value of i, $\Gamma_{il} = 0$. Since all parameters in (10.109) are positive, Γ_{il} can only vanish if

$$i_{\max} + l + 1 = \lambda$$

The function u so generated is a polynomial and, due to the exponential term in the form (10.107), we see that, as demanded, the wavefunction is finite everywhere.

Since i and l are integers, it follows that λ is also an integer, which is called the *principal quantum number*, n.

$$n = i_{\max} + l + 1$$

Thus the above cutoff condition on the series (10.107), which ensures that $u(\rho)$ is finite for all ρ, also serves to determine the eigenenergies λ.

$$\lambda_n{}^2 = n^2 = \frac{Z^2 \mathbb{R}}{|E_n|}$$

$$\boxed{E_n = -|E_n| = -\frac{Z^2 \mathbb{R}}{n^2}} \tag{10.110}$$

These are the same values found previously in the simpler Bohr model (Section 2.4).

Laguerre Polynomials

The hydrogen eigenfunction corresponding to the eigenvalue E_n is given by (10.107) with the series over i cut off at the value

$$i_{\max} = n - l - 1 \tag{10.111}$$

and the recurrence relation for the coefficients $\{C_i\}$ given by (10.109).

$$\begin{gathered} u_{nl}(\rho) = e^{-\rho/2}\rho^{l+1}F_{nl}(\rho) = A_{nl}e^{-\rho/2}\rho^{l+1}\sum_{i=0}^{n-l-1} C_i\rho^i \\ C_{i+1} = \Gamma_{il}C_i, \qquad \rho \equiv 2\kappa_n r, \qquad \kappa_n = \frac{Z}{a_0 n} \end{gathered} \tag{10.112}$$

where A_{nl} is a normalization constant. The polynomials $F_{nl}(\rho)$ (of order $n - l - 1$) so obtained are better known as the *associated Laguerre polynomials*, L_{n-l-1}^{2l+1} (see Table 10.3). The reader should take note of the fact that the scale of length ρ changes

TABLE 10.3 Eigenfunctions of hydrogen in terms of associated Laguerre polynomials

The Normalized Eigenfunctions of Hydrogen ($Z = 1$)

$$\varphi_{nlm}(r, \theta, \phi) = (2\kappa)^{3/2}A_{nl}\rho^l e^{-\rho/2}F_{nl}(\rho)Y_l^m(\theta, \phi) = R_{nl}(r)Y_l^m(\theta, \phi)$$

$$\rho = 2\kappa r = \frac{2Z}{a_0 n}r \qquad \int_0^\infty |R_{nl}(r)|^2 r^2\, dr = 1$$

$$A_{nl} = \sqrt{\frac{(n-l-1)!}{2n[(n+l)!]^3}} \qquad \boxed{\varphi_{100} = \frac{1}{\sqrt{8\pi}}\left(\frac{2Z}{a_0}\right)^{3/2} e^{-(Z/a_0)r}}$$

$$F_{nl}(\rho) = L_{n-l-1}^{2l+1}(\rho) = L_{i_{\max}}^{2l+1}(\rho) = \sum_{i=0}^{n-l-1} \frac{(-1)^i[(n+l)!]^2\rho^i}{i!(n-l-1-i)!(2l+1+i)!}$$

Associated Laguerre Polynomials $L_p^q(\rho)$ *and Laguerre Polynomials* $L_p(\rho)$

Differential equation:

$$\left[\rho\frac{d^2}{d\rho^2} + (q + 1 - \rho)\frac{d}{d\rho} + p\right]L_p^q(\rho) = 0$$

Generating function:

$$\frac{e^{-\rho s/(1-s)}}{(1-s)^{q+1}} = \sum_{p=0}^\infty \frac{s^p}{(p+q)!}L_p^q(\rho), \qquad L_0^p(0) = p!$$

Orthonormality:

$$\int_0^\infty e^{-\rho}\rho^q L_p^q L_{p'}^q\, d\rho = \frac{[(p+q)!]^3}{p!}\delta_{pp'}$$

(*Continued*)

TABLE 10.3 *(Continued)*

Rodrigues' formula:

$$L_p(\rho) \equiv L_p^0(\rho) = e^\rho \frac{d^p}{d\rho^p}(\rho^p e^{-\rho}), \qquad L_1(\rho) = 1 - \rho, \qquad L_2(\rho) = 2!\left(1 - 2\rho + \frac{\rho^2}{2}\right)$$

$$L_p^q(\rho) \equiv (-1)^q \frac{d^q}{d\rho^q}[L_{q+p}(\rho)]$$

Recurrence relations:

$$\rho L_p^q(\rho) = (2p + q + 1)L_p^q(\rho) - [(p + 1)/(p + q + 1)]L_{p+1}^q(\rho) - (p + q)^2 L_{p-1}^q(\rho)$$

$$\left(\rho \frac{d}{d\rho} + q - \rho\right)L_p^q(\rho) = (p + 1)L_{p+1}^{q-1}(\rho)$$

$$\frac{d}{d\rho} L_p^q(\rho) = -L_{p-1}^{q+1}(\rho)$$

Relation to Other Notations

Alternative notations for the polynomial L_p^q may be found in other texts. The relation between this notation (B) and our own (A) is given by the following table.[a]

Notation A (e.g., found in Merzbacher, Messiah, and here)	Notation B (e.g., found in Pauling and Wilson, Schiff, and Tomonaga)
$(-)^q L_p^q$	L_{p+q}^q
$\rho(L_p^q)'' + (q + 1 - \rho)(L_p^q)' + pL_p^q = 0$	$\rho(L_{p+q}^q)'' + (q + 1 - \rho)(L_{p+q}^q)' + pL_{p+q}^q = 0$
$R_{nl} = A(2\kappa)^{3/2} e^{-\rho/2} \rho^l L_{n-l-1}^{2l-1}(\rho)$	$R_{nl} = -A(2\kappa)^{3/2} e^{-\rho/2} \rho^l L_{n+l}^{2l+1}(\rho)$
L_p^q is a polynomial of order p	L_{p+q}^q is a polynomial of order p or, equivalently, L_b^a is a polynomial of order $(b - a)$

The first row in this table tells us that L_p^q is written L_{p+q}^q in notation B. The second row indicates that both L functions satisfy the same differential equation. The third row gives the forms of the radial solution R_{nl} in both notations. Still another notation appears in I. S. Gradshteyn and I. M. Ryzhik,[b] where

$$L_p^q(\rho)[\text{here}] = (p + q)!L_p^q(\rho)[\text{G and R}]$$

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[a] E. Merzbacher, *Quantum Mechanics*, 2nd ed., Wiley, New York, 1970.
A. Messiah, *Quantum Mechanics*, Wiley, New York, 1966.
L. Pauling and E. B. Wilson, *Introduction to Quantum Mechanics*, McGraw-Hill, New York, 1935.
L. Schiff, *Quantum Mechanics*, 3rd ed., McGraw-Hill, New York, 1968.
S. Tomanaga, *Quantum Mechanics*, North-Holland, Amsterdam, 1966.

[b] I. S. Gradshteyn and I. M. Ryzhik, *Tables of Integrals, Series and Products*, Academic Press, New York, 1965.

with different values of n. This is due to the radial displacement r being nondimensionalized through the wavenumber κ_n, which is dependent on n.

Degeneracy

Since $i_{\max} \geq 0$, with (10.111) we obtain

$$l \leq n - 1$$

So for a given value of the *principal quantum number n*, the *orbital quantum number l* cannot exceed the value

$$l_{\max} = n - 1 \tag{10.113}$$

This corresponds to the values $l = 0, 1, 2, \ldots, (n - 1)$. Each of these l values corresponds to different values of $i_{\max}$ and therefore different wavefunctions. Inasmuch as the eigenenergy E_n depends only on the principal quantum number n, these n distinct orbital states are degenerate. For instance, there are three distinct radial functions that correspond to the eigenenergy E_3. These are $u_{3,0}$, $u_{3,1}$, and $u_{3,2}$.

The complete eigenstate of the Hamiltonian (10.101) contains the factor $Y_l^m(\theta, \phi)$ [see (10.94)]. For each value of l, there are $2l + 1$ values of m_l: $m_l = -l, \ldots, +l$, which correspond to distinct Y_l^m functions that give the same eigenvalues of $\hat{L}^2$ [i.e., $\hbar^2 l(l + 1)$]. All these $2l + 1$ functions when substituted into (10.102) give the same radial equation, (10.103), which contains only the orbital number l. It follows that for each solution u_{nl} of (10.106), there are $(2l + 1)$ solutions to the Schrödinger equation (10.102) corresponding to the same eigenenergy E_n (see Table 10.4). In this manner we obtain

$$\text{degeneracy of } E_n = \sum_{l=0}^{n-1} (2l + 1) = n^2 \tag{10.114}$$

TABLE 10.4 Allowed values of l and m_l for $n = 1, 2, 3$

n	1	2		3		
l	0	0	1	0	1	2
Spectroscopic notation of state	1*S*	2*S*	2*P*	3*S*	3*P*	3*D*
m_l	0	0	$-1, 0, +1$	0	$-1, 0, +1$	$-2, -1, 0, +1, +2$
Degeneracy of state (n^2)	1	4		9		

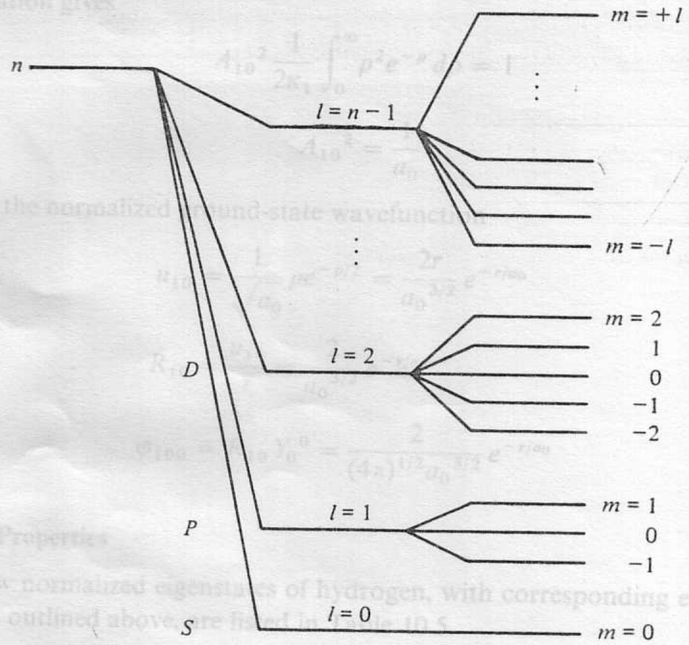

FIGURE 10.13 Term diagram for a hydrogenic atom illustrating all n^2 degenerate states corresponding to the principal quantum number n.

To recapitulate, the allowed values of n, l, and m are (see Fig. 10.13)

$$\begin{aligned} n &= 1, 2, 3, \ldots \\ l &= 0, 1, 2, \ldots, (n-1) \qquad (10.115) \\ m &= -l, -l+1, \ldots, 0, 1, 2, \ldots, +l \end{aligned}$$

Additional Properties of the Eigenstates

The eigenfunctions and eigenenergies of the hydrogenic Hamiltonian (10.101) are

$$\boxed{\begin{aligned} \varphi_{nlm}(r, \theta, \phi) &= R_{nl}(r) Y_l^m(\theta, \phi) \\ R_{nl} &= \frac{A_{nl} u_{nl}}{r} \\ E_n = -\frac{Z^2 \mathbb{R}}{n^2} &= -\frac{\mu (Ze^2)^2}{2\hbar^2 n^2} \end{aligned}} \qquad (10.116)$$

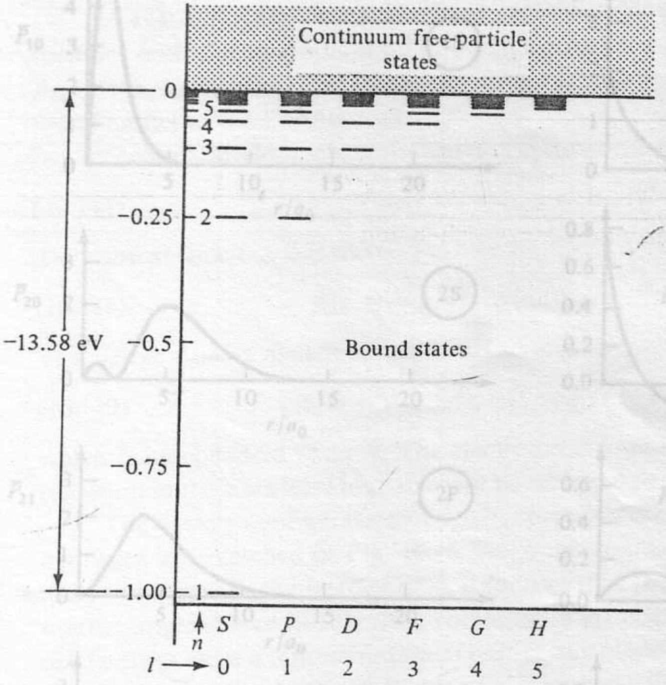

FIGURE 10.14 Energy-level diagram for hydrogen, including the $l \le 5$ terms. Energy is measured in units of $\mathbb{R}$.

A term diagram of these energies is given in Fig. 10.14 (compare Fig. 2.8). The normalization constant A_{nl} (see Table 10.3) is determined by the condition

$$\langle \varphi_{nlm} | \varphi_{nlm} \rangle = \int_{4\pi} d\Omega \int_0^\infty r^2\, dr\, \varphi_{nlm}{}^* \varphi_{nlm}$$

$$= |A_{nl}|^2 \int_0^\infty |u_{nl}|^2\, dr = 1$$

Note also the orthogonality of these functions

$$\langle \varphi_{n'l'm'} | \varphi_{nlm} \rangle = \delta_{nn'}\, \delta_{ll'}\, \delta_{mm'}$$

The Ground State

To construct the *ground state* φ_{100} ($n = 1$, $l = 0$, $m = 0$) we must first find u_{10}. From (10.112), with $C_0 = 1$, and inserting the normalization constant[1] A_{10}, one obtains

$$u_{10} = A_{10} e^{-\rho/2} \rho$$

---

[1] Alternatively, we may take $C_0 = A_{10}$.

Normalization gives

$$A_{10}{}^2 \frac{1}{2\kappa_1} \int_0^\infty \rho^2 e^{-\rho}\, d\rho = 1$$

$$A_{10}{}^2 = \frac{1}{a_0}$$

This gives the normalized ground-state wavefunction

$$u_{10} = \frac{1}{\sqrt{a_0}} \rho e^{-\rho/2} = \frac{2r}{a_0{}^{3/2}} e^{-r/a_0}$$

$$R_{10} = \frac{u_{10}}{r} = \frac{2}{a_0{}^{3/2}} e^{-r/a_0}$$

$$\varphi_{100} = R_{10}\, Y_0{}^0 = \frac{2}{(4\pi)^{1/2} a_0{}^{3/2}} e^{-r/a_0}$$

Additional Properties

The first few normalized eigenstates of hydrogen, with corresponding eigenenergies obtained as outlined above, are listed in Table 10.5.

TABLE 10.5

Spectroscopic Notation	Several Normalized Time-Independent Eigenstates of Hydrogen
$1S$	$\varphi_{100} = \frac{2}{a_0{}^{3/2}} e^{-r/a_0} Y_0{}^0(\theta, \phi)$
$2S$	$\varphi_{200} = \frac{2}{(2a_0)^{3/2}} (1 - r/2a_0) e^{-r/2a_0} Y_0{}^0(\theta, \phi)$
$2P$	$\begin{pmatrix} \varphi_{211} \\ \varphi_{210} \\ \varphi_{21-1} \end{pmatrix} = \frac{1}{\sqrt{3}(2a_0)^{3/2}} \frac{r}{a_0} e^{-r/2a_0} \begin{pmatrix} Y_1{}^1(\theta, \phi) \\ Y_1{}^0(\theta, \phi) \\ Y_1{}^{-1}(\theta, \phi) \end{pmatrix}$
$3S$	$\varphi_{300} = \frac{2}{3(3a_0)^{3/2}} [3 - 2r/a_0 + 2(r/3a_0)^2] e^{-r/3a_0} Y_0{}^0(\theta, \phi)$
$3P$	$\begin{pmatrix} \varphi_{311} \\ \varphi_{310} \\ \varphi_{31-1} \end{pmatrix} = \frac{4\sqrt{2}}{9(3a_0)^{3/2}} \frac{r}{a_0} (1 - r/6a_0) e^{-r/3a_0} \begin{pmatrix} Y_1{}^1(\theta, \phi) \\ Y_1{}^0(\theta, \phi) \\ Y_1{}^{-1}(\theta, \phi) \end{pmatrix}$
$3D$	$\begin{pmatrix} \varphi_{322} \\ \varphi_{321} \\ \varphi_{320} \\ \varphi_{32-1} \\ \phi_{32-2} \end{pmatrix} = \frac{2\sqrt{2}}{27\sqrt{5}(3a_0)^{3/2}} \left(\frac{r}{a_0}\right)^2 e^{-r/3a_0} \begin{pmatrix} Y_2{}^2(\theta, \phi) \\ Y_2{}^1(\theta, \phi) \\ Y_2{}^0(\theta, \phi) \\ Y_2{}^{-1}(\theta, \phi) \\ Y_2{}^{-2}(\theta, \phi) \end{pmatrix}$

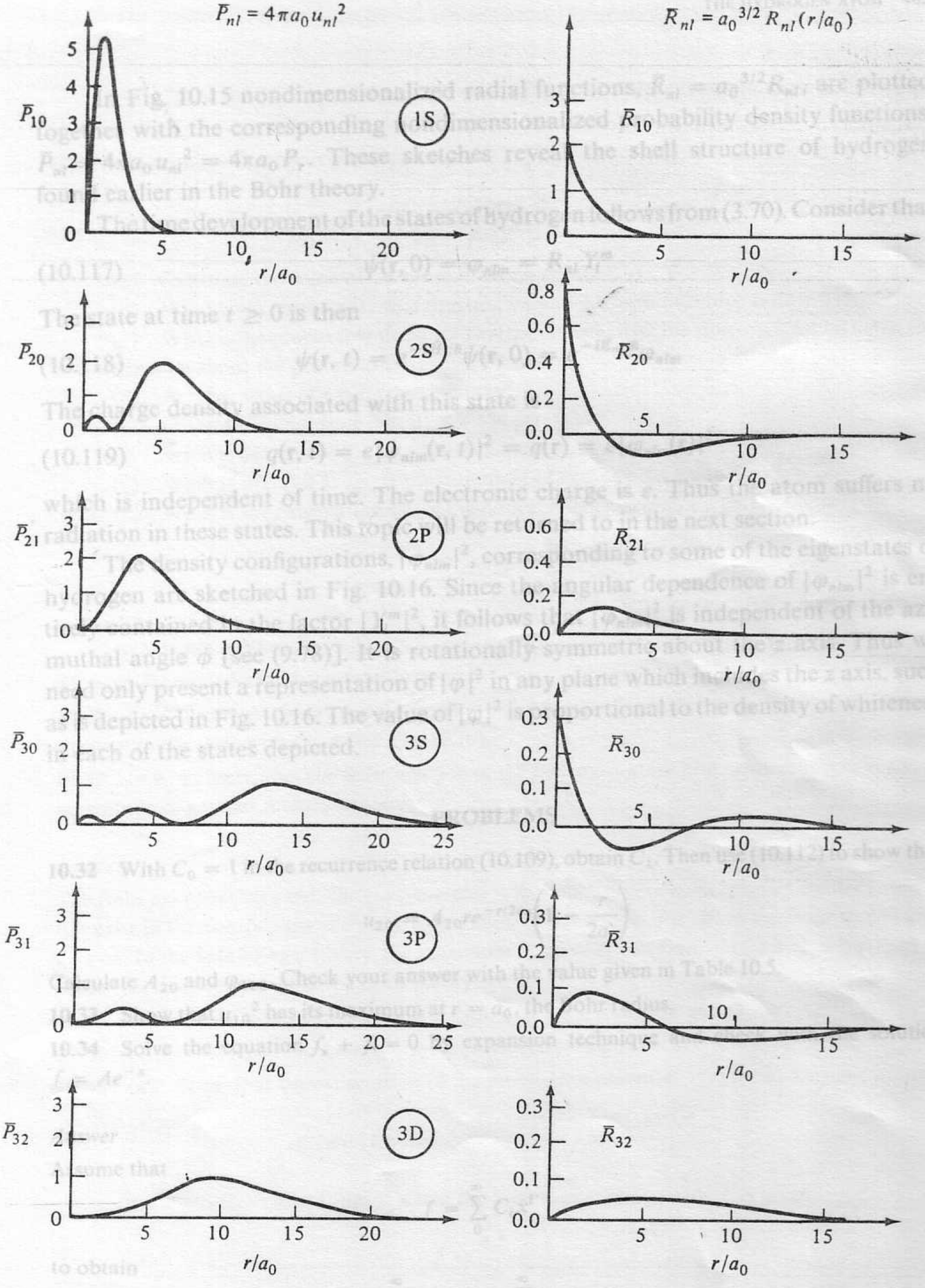

FIGURE 10.15 **Nondimensional radial probability density $\bar{P}$ and nondimensional radial wavefunction $\bar{R}$, vs. nondimensional radius r/a_0, for hydrogen. Note that the probability density $\bar{P}$ exhibits the shell structure of the atom.**

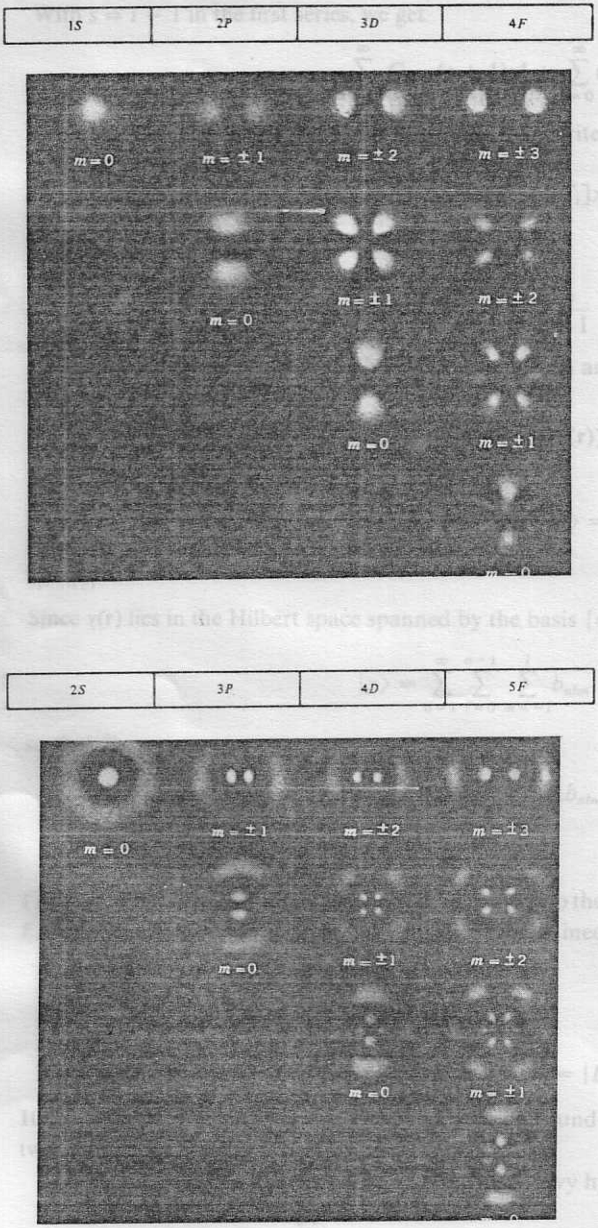

FIGURE 10.16 Probability density, $|\varphi_{nlm}|^2$, for various states of hydrogen. The plane of the paper contains the polar axis, which points from the bottom to the top of the figure. From *Principles of Modern Physics* by R. B. Leighton. Copyright 1959 by McGraw-Hill. Used with permission of the McGraw-Hill Book Company.

In Fig. 10.15 nondimensionalized radial functions, $\bar{R}_{nl} = a_0^{3/2} R_{nl}$, are plotted together with the corresponding nondimensionalized probability density functions, $\bar{P}_{nl} = 4\pi a_0 u_{nl}^2 = 4\pi a_0 P_r$. These sketches reveal the shell structure of hydrogen found earlier in the Bohr theory.

The time development of the states of hydrogen follows from (3.70). Consider that

$$\psi(\mathbf{r}, 0) = \varphi_{nlm} = R_{nl} Y_l^m \tag{10.117}$$

The state at time $t \geq 0$ is then

$$\psi(\mathbf{r}, t) = e^{-i\hat{H}t/\hbar}\psi(\mathbf{r}, 0) = e^{-iE_n t/\hbar}\varphi_{nlm} \tag{10.118}$$

The charge density associated with this state is

$$q(\mathbf{r}, t) = e|\psi_{nlm}(\mathbf{r}, t)|^2 = q(\mathbf{r}) = e|\varphi_{nlm}(\mathbf{r})|^2 \tag{10.119}$$

which is independent of time. The electronic charge is e. Thus the atom suffers no radiation in these states. This topic will be returned to in the next section.

The density configurations, $|\varphi_{nlm}|^2$, corresponding to some of the eigenstates of hydrogen are sketched in Fig. 10.16. Since the angular dependence of $|\varphi_{nlm}|^2$ is entirely contained in the factor $|Y_l^m|^2$, it follows that $|\varphi_{nlm}|^2$ is independent of the azimuthal angle ϕ [see (9.78)]. It is rotationally symmetric about the z axis. Thus we need only present a representation of $|\varphi|^2$ in any plane which includes the z axis, such as is depicted in Fig. 10.16. The value of $|\varphi|^2$ is proportional to the density of whiteness in each of the states depicted.

PROBLEMS

10.32 With $C_0 = 1$ in the recurrence relation (10.109), obtain C_1. Then use (10.112) to show that

$$u_{20} = A_{20} r e^{-r/2a_0}\left(1 - \frac{r}{2a_0}\right)$$

Calculate A_{20} and φ_{200}. Check your answer with the value given in Table 10.5.

10.33 Show that u_{10}^2 has its maximum at $r = a_0$, the Bohr radius.

10.34 Solve the equation $f_x + f = 0$ by expansion technique and check with the solution $f = Ae^{-x}$.

Answer

Assume that

$$f = \sum_0^\infty C_i x^i$$

to obtain

$$\sum_0^\infty C_i i x^{i-1} + \sum_0^\infty C_i x^i = 0$$

With $s = i - 1$ in the first series, we get

$$\sum_{s=-1}^{\infty} C_{s+1}(s+1)x^s + \sum_{i=0}^{\infty} C_i x^i = 0$$

Since the first term in the first series is zero, we may write this equation in the form

$$\sum_{i=0}^{\infty} [C_{i+1}(i+1) + C_i]x^i = 0$$

which is satisfied if and only if

$$C_{i+1} = -\frac{C_i}{i+1}$$

10.35 The average energy of the hydrogen atom in an arbitrary bound state $\chi(\mathbf{r})$ is given by the integral

$$\langle E \rangle = \langle \chi(\mathbf{r}) | \hat{H} | \chi(\mathbf{r}) \rangle$$

Show that

$$\langle E \rangle \geq \langle 100 | \hat{H} | 100 \rangle = E_1$$

Answer

Since $\chi(\mathbf{r})$ lies in the Hilbert space spanned by the basis $\{\varphi_{nlm}\}$, we may expand

$$|\chi\rangle = \sum_{n=1}^{\infty} \sum_{l=0}^{n-1} \sum_{m=-l}^{l} b_{nlm} |nlm\rangle$$

so that

$$\langle \chi | \hat{H} | \chi \rangle = \sum_n \sum_l \sum_m |b_{nlm}|^2 E_n$$

$$\sum \sum \sum |b|^2 = 1$$

(The ket vector $|nlm\rangle$ represents the state φ_{nlm}.) Owing to the fact that all eigenenergies are negative, $E_n \leq 0$. the statement to be proven is equivalent to the inequality

$$\begin{aligned} |\langle E \rangle| &\leq |E_1| \\ |\langle E \rangle| &= \sum \sum \sum |b|^2 |E_n| \\ &\leq |E|_{\max} \sum \sum \sum |b|^2 = |E|_{\max} = |E_1| \end{aligned}$$

10.36 (a) What is the effective Bohr radius and ground-state energy for each of the following two-particle systems?

(1) H^2, a deuteron and an electron (heavy hydrogen).

(2) He^+, a singly ionized helium.

(3) Positronium, a bound positron and electron.

(4) Mesonium, a proton and negative μ meson. The μ meson has mass $207m_e$ and lasts $\sim 10^{-6}$ s.

(5) Two neutrons bound together by their gravitational field.

(b) Calculate the frequencies of the $(n = 2) \rightarrow (n = 1)$ transition for each of the systems above.

10.37 At time $t = 0$, a hydrogen atom is in the superposition state

$$\psi(\mathbf{r}, 0) = \frac{4}{(2a_0)^{3/2}}\left[e^{-r/a_0} + A\frac{r}{a_0}e^{-r/2a_0}(-iY_1{}^1 + Y_1{}^{-1} + \sqrt{7}\,Y_1{}^0)\right]$$

(a) Calculate the value of the normalization constant A.
(b) What is the probability that measurement of L^2 finds the value $\hbar^2 l(l+1)$?
(c) What is the probability density $P_r(r)$ [see (10.99)] that the electron is found in the shell of thickness dr about the proton at the radius r?
(d) At what value of r is $P_r(r)$ maximum?
(e) Given the initial state $\psi(\mathbf{r}, 0)$, what is $\psi(\mathbf{r}, t)$?
(f) What is $\psi(\mathbf{r}, t)$ if at $t = 0$, measurement of L_z finds the value $\hbar$?
(g) What is $\psi(\mathbf{r}, t)$ if at $t = 0$, measurement of L_z finds the value zero?
(h) What is the expectation of the "spherical energy operator," $\langle H_S\rangle$, where

$$\hat{H}_S \equiv \hat{H} - \frac{\hat{p}_r{}^2}{2\mu}$$

at $t = 0$?

(i) What is the lowest value of energy that measurement will find at $t = 0$? (Lowest means the negative value farthest removed from zero.)

10.38 Find the lowest energy and the smallest value for the classical turning radius of the H-atom electron in the state with $l = 6$ (see Fig. 10.10).

10.39 In what sense does the Bohr analysis of the hydrogen atom give erroneous results for the magnitude of angular momentum, L?

Answer

The Bohr analysis that yields the eigenenergies $-\mathbb{R}/n^2$ assumes circular orbits. Circular orbits do not exist in the Schrödinger theory. Quantization of the action, $\oint p_\theta\, d\theta$, in the Bohr theory gives $L = n\hbar$. In the Schrödinger theory, the maximum value of L is $\hbar\sqrt{n(n-1)}$, which is less than the value that L assumes $(n\hbar)$ in the Bohr theory.

10.40 What is the ionization energy of a hydrogen atom in the $3P$ state?

10.41 Show that $R_{nl}(r)$ has $(n - l - 1)$ zeros (not counting zeros at $r = 0$ and $r = \infty$).

10.42 (a) Show that the expectation of the interaction potential $V(r)$ for hydrogenic atoms is

$$\langle nlm|V(r)|nlm\rangle = -\left\langle\frac{Ze^2}{r}\right\rangle = -\frac{\mu Z^2 e^4}{\hbar^2 n^2}$$

(b) Calculate $\langle nlm|\hat{T}|nlm\rangle$, where the kinetic-energy operator $\hat{T}$ is given

$$\hat{T} = \frac{\hat{p}_r{}^2}{2\mu} + \frac{\hat{L}^2}{2\mu r^2}$$

What relation do $\langle T\rangle$ and $\langle V\rangle$ satisfy? (*The virial theorem.*)

10.43 Obtain an explicit expression for the probability density $P_r(r)$ corresponding to the state whose energy is E_2, for a hydrogenic atom [see (10.99)].

Answer

There are four degenerate eigenstates corresponding to the energy E_2. Since no direction is preferred for a Hamiltonian whose only interaction term is the central potential $V(r)$, all these degenerate states carry the same "weight" (all lm states are equally probable). There results

$$
\begin{aligned}
4\pi P(r) r^2\, dr &= \int_{4\pi} \frac{1}{4}[\varphi_{200}{}^*\varphi_{200} + \varphi_{21-1}{}^*\varphi_{21-1} + \varphi_{210}{}^*\varphi_{210} + \varphi_{211}{}^*\varphi_{211}]r^2\, dr\, d\Omega \\
&= \int_{4\pi} \frac{1}{128\pi}\left(\frac{Z}{a_0}\right)^3 e^{-Zr/a}\left[\left(2-\frac{Zr}{a_0}\right)^2 + \left(\frac{Zr}{a_0}\right)^2\left(\frac{1}{2}\sin^2\theta + \frac{1}{2}\sin^2\theta + \cos^2\theta\right)\right] \\
&\quad \times r^2\, dr\, d\Omega
\end{aligned}
$$

$$
P(r) = \frac{1}{128\pi}\left(\frac{Z}{a_0}\right)^3 e^{-Zr/a_0}\left[\left(2-\frac{Zr}{a_0}\right)^2 + \left(\frac{Zr}{a_0}\right)^2\right], \qquad P_r(r) = 4\pi r^2 P(r)
$$

10.44 Give a physical argument in support of the conjecture that the sum

$$
\sum\nolimits_n \equiv \sum_{l=0}^{n-1}\sum_{m=-l}^{+l}[Y_l^m]^*[Y_l^m][R_{nl}]^2
$$

is independent of θ or ϕ.

10.45 Show that for a hydrogen atom in the state corresponding to maximum orbital angular momentum ($l = n - 1$),

$$
\langle n, n-1|r|n, n-1\rangle = a_0 n(n + \tfrac{1}{2})
$$

$$
\langle n, n-1|r^2|n, n-1\rangle = a_0{}^2 n^2(n+1)(n + \tfrac{1}{2})
$$

10.46 Use the results of Problem 10.45 to show that for large values of n and l,

$$
\sqrt{\langle r^2\rangle} \to a_0 n^2
$$

$$
\frac{\Delta r}{\langle r\rangle} \to 0
$$

$$
E_n \to -\frac{1}{2}\frac{e^2}{n^2 a_0}
$$

That is, show that for large values of n, the electron is localized near the surface of a sphere of radius $a_0 n^2$ and has energy which is the same as that of a classical electron in a circular orbit of the same radius. Recall: $(\Delta r)^2 = \langle r^2\rangle - \langle r\rangle^2$.

10.47 Calculate $\langle \mathbf{r} \rangle$ in the state φ_{nlm} of hydrogen.

Answer

$$\langle \mathbf{r} \rangle = \mathbf{e}_x \langle x \rangle + \mathbf{e}_y \langle y \rangle + \mathbf{e}_z \langle z \rangle$$

$$\langle x \rangle = \iiint r \cos\phi \sin\theta \, |Y_l^m|^2 R_{nl}{}^2 r^2 \, dr \, d\cos\theta \, d\phi$$

$$= 0$$

since

$$\int_0^{2\pi} \cos\phi \, d\phi = 0$$

and $|Y_l^m|^2$ is independent of ϕ. Similarly, $\langle y \rangle = 0$. For $\langle z \rangle$ we must calculate

$$\langle z \rangle = \int_{-1}^{1} |P_l{}^m|^2 \cos\theta \, d\cos\theta \int \cdots$$

Using the recurrence relations listed in Table 9.3, we find that $\langle z \rangle = 0$. It follows that $\langle \mathbf{r} \rangle = 0$.

10.48 Establish the following properties for hydrogen in the stationary state φ_{nlm}.

(a) $\dfrac{s+1}{n^2}\langle r^s \rangle - (2s+1)a_0\langle r^{s-1} \rangle + \dfrac{s}{4}[(2l+1)^2 - s^2]a_0{}^2\langle r^{s-2} \rangle = 0, \quad s > -2l-1$

(b) $\langle r \rangle = n^2\left[1 + \dfrac{1}{2}\left(1 - \dfrac{l(l+1)}{n^2}\right)\right]a_0$

(c) $\left\langle \dfrac{1}{r^2} \right\rangle = \dfrac{2}{(2l+1)n^3 a_0{}^2}$

(d) $\langle r^2 \rangle = \dfrac{1}{2}[5n^2 + 1 - 3l(l+1)]n^2 a_0{}^2$

(e) $\left\langle \dfrac{1}{r} \right\rangle = \dfrac{1}{n^2 a_0}$

(f) $\left\langle \dfrac{1}{r^3} \right\rangle = \dfrac{2}{a_0{}^3 n^3 l(l+1)(2l+1)}$

[*Hint*: Multiply (10.106) by $\{\rho^{s+1}u' + [(s+1)/2]\rho\}$ and integrate by parts several times. Note that for hydrogenic atoms, a_0 is replaced by a_0/Z.]

10.49 Show that the most probable values of r for the $l = n-1$ states of hydrogen are

$$\tilde{r} = n^2 a_0$$

These are values that satisfy the equation

$$\frac{d}{dr}(u_{nl})^2 = 0$$